



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2026 – 12:05 PM UTC

PDB ID : 2RH7 / pdb_00002rh7
Title : Crystal Structures of the Luciferase and Green Fluorescent Protein from Renilla Reniformis
Authors : Loening, A.M.; Fenn, T.D.; Gambhir, S.S.
Deposited on : 2007-10-06
Resolution : 1.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

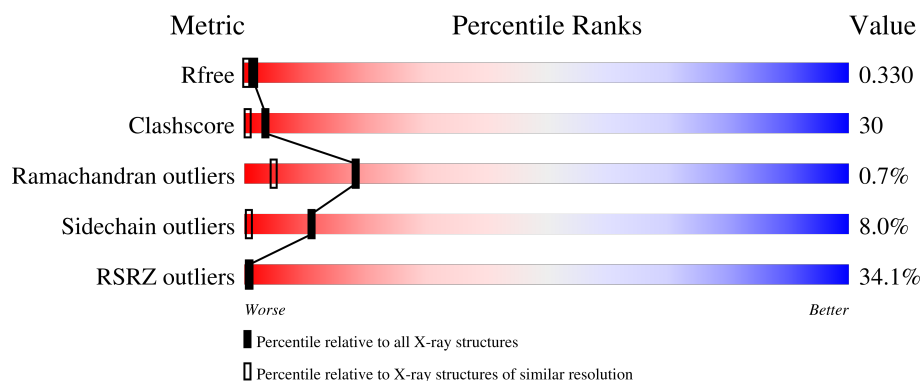
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (1.50-1.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	239	
1	B	239	
1	C	239	
1	D	239	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	CRO	A	66	-	-	X	-
1	CRO	B	66	-	-	X	-
1	CRO	C	66	-	-	X	-
1	CRO	D	66	-	-	X	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7391 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Green fluorescent protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	212	Total	C	N	O	S	0	3	0
			1714	1100	283	320	11			
1	B	213	Total	C	N	O	S	0	4	0
			1733	1110	285	329	9			
1	C	212	Total	C	N	O	S	0	1	0
			1700	1092	281	318	9			
1	D	212	Total	C	N	O	S	0	2	0
			1707	1097	283	317	10			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	66	CRO	SER	chromophore	UNP Q963I9
A	66	CRO	TYR	chromophore	UNP Q963I9
A	66	CRO	GLY	chromophore	UNP Q963I9
A	234	VAL	-	expression tag	UNP Q963I9
A	235	ASP	-	expression tag	UNP Q963I9
A	236	HIS	-	expression tag	UNP Q963I9
A	237	HIS	-	expression tag	UNP Q963I9
A	238	HIS	-	expression tag	UNP Q963I9
A	239	HIS	-	expression tag	UNP Q963I9
A	240	HIS	-	expression tag	UNP Q963I9
A	241	HIS	-	expression tag	UNP Q963I9
B	66	CRO	SER	chromophore	UNP Q963I9
B	66	CRO	TYR	chromophore	UNP Q963I9
B	66	CRO	GLY	chromophore	UNP Q963I9
B	234	VAL	-	expression tag	UNP Q963I9
B	235	ASP	-	expression tag	UNP Q963I9
B	236	HIS	-	expression tag	UNP Q963I9
B	237	HIS	-	expression tag	UNP Q963I9
B	238	HIS	-	expression tag	UNP Q963I9
B	239	HIS	-	expression tag	UNP Q963I9
B	240	HIS	-	expression tag	UNP Q963I9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	241	HIS	-	expression tag	UNP Q963I9
C	66	CRO	SER	chromophore	UNP Q963I9
C	66	CRO	TYR	chromophore	UNP Q963I9
C	66	CRO	GLY	chromophore	UNP Q963I9
C	234	VAL	-	expression tag	UNP Q963I9
C	235	ASP	-	expression tag	UNP Q963I9
C	236	HIS	-	expression tag	UNP Q963I9
C	237	HIS	-	expression tag	UNP Q963I9
C	238	HIS	-	expression tag	UNP Q963I9
C	239	HIS	-	expression tag	UNP Q963I9
C	240	HIS	-	expression tag	UNP Q963I9
C	241	HIS	-	expression tag	UNP Q963I9
D	66	CRO	SER	chromophore	UNP Q963I9
D	66	CRO	TYR	chromophore	UNP Q963I9
D	66	CRO	GLY	chromophore	UNP Q963I9
D	234	VAL	-	expression tag	UNP Q963I9
D	235	ASP	-	expression tag	UNP Q963I9
D	236	HIS	-	expression tag	UNP Q963I9
D	237	HIS	-	expression tag	UNP Q963I9
D	238	HIS	-	expression tag	UNP Q963I9
D	239	HIS	-	expression tag	UNP Q963I9
D	240	HIS	-	expression tag	UNP Q963I9
D	241	HIS	-	expression tag	UNP Q963I9

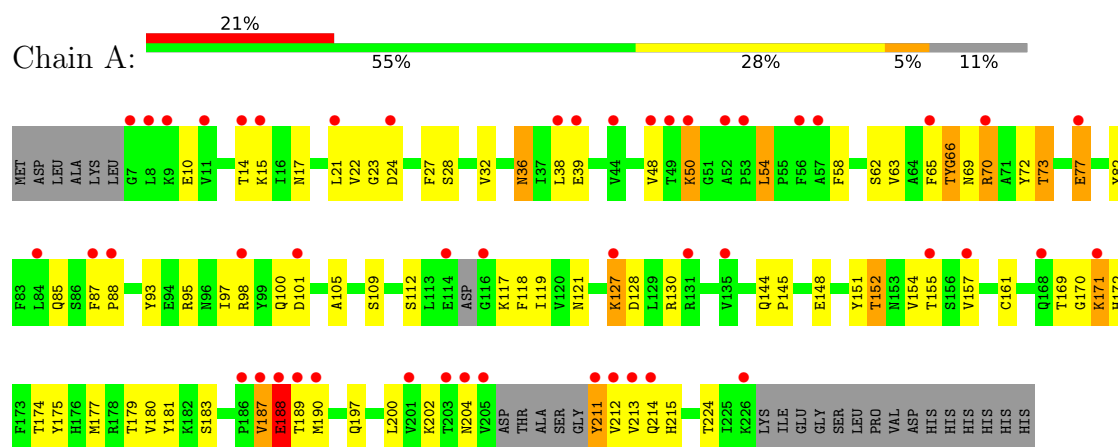
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	132	Total O 132 132	0	0
2	B	138	Total O 138 138	0	0
2	C	146	Total O 146 146	0	0
2	D	121	Total O 121 121	0	0

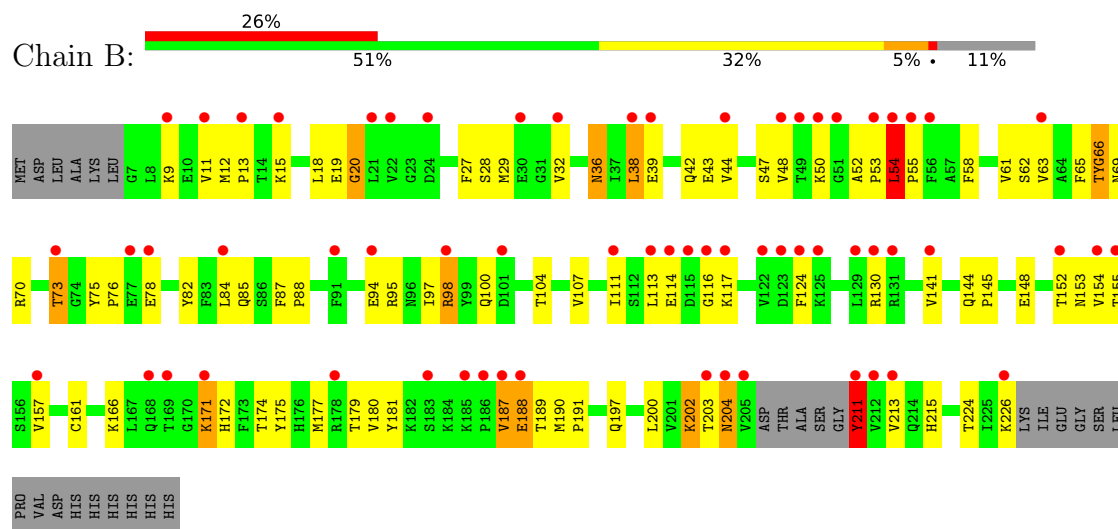
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

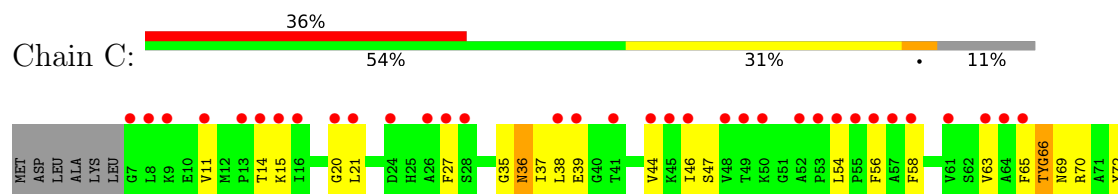
• Molecule 1: Green fluorescent protein



• Molecule 1: Green fluorescent protein



• Molecule 1: Green fluorescent protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	73.74Å 85.41Å 158.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.50 50.00 – 1.50	Depositor EDS
% Data completeness (in resolution range)	76.8 (50.00-1.50) 87.0 (50.00-1.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.291 , 0.325 0.301 , 0.330	Depositor DCC
R_{free} test set	7018 reflections (4.35%)	wwPDB-VP
Wilson B-factor (Å ²)	(Not available)	Xtriage
Anisotropy	(Not available)	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 69.8	EDS
L-test for twinning ¹	$\langle L \rangle =$ (Not available), $\langle L^2 \rangle =$ (Not available)	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7391	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *(Not available)*

¹Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CRO

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.44	0/1728	0.81	1/2330 (0.0%)
1	B	0.46	0/1748	0.80	4/2359 (0.2%)
1	C	0.43	0/1714	0.83	4/2311 (0.2%)
1	D	0.46	0/1722	0.87	4/2322 (0.2%)
All	All	0.45	0/6912	0.83	13/9322 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	211	TYR	N-CA-C	-11.96	95.14	111.28
1	C	211	TYR	N-CA-C	-7.91	88.84	111.00
1	D	114	GLU	N-CA-C	6.90	124.38	114.16
1	A	211	TYR	N-CA-C	-6.83	91.87	111.00
1	B	54	LEU	CA-C-N	6.47	127.03	120.04
1	B	54	LEU	C-N-CA	6.47	127.03	120.04
1	B	20	GLY	N-CA-C	6.28	122.44	111.14
1	B	211	TYR	N-CA-C	-6.22	93.59	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	212	VAL	N-CA-C	6.20	117.95	108.71
1	D	212	VAL	N-CA-C	5.99	118.26	109.63
1	C	54	LEU	CA-C-N	5.27	126.30	120.45
1	C	54	LEU	C-N-CA	5.27	126.30	120.45
1	D	144	GLN	N-CA-C	-5.03	102.85	110.50

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	211	TYR	Peptide
1	B	211	TYR	Peptide
1	C	211	TYR	Peptide
1	D	211	TYR	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1714	0	1689	94	0
1	B	1733	0	1698	124	0
1	C	1700	0	1676	94	0
1	D	1707	0	1689	122	0
2	A	132	0	0	11	0
2	B	138	0	0	16	0
2	C	146	0	0	10	0
2	D	121	0	0	9	0
All	All	7391	0	6752	407	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 30.

All (407) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:ARG:HH11	1:A:70:ARG:HG2	1.04	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:TYR:HE2	1:B:177:MET:HE3	1.12	1.10
1:C:14:THR:HG22	1:C:118:PHE:HB2	1.33	1.10
1:A:14:THR:HG22	1:A:118:PHE:HB2	1.20	1.09
1:D:14:THR:HG22	1:D:118:PHE:HB2	1.28	1.07
1:A:65:PHE:C	1:A:66:CRO:N1	2.18	1.02
1:D:152:THR:HG21	1:D:190:MET:HB3	1.36	1.02
1:A:48:VAL:HG21	1:A:54:LEU:HD11	1.43	1.00
1:B:48:VAL:HG21	1:B:54:LEU:HD11	1.43	1.00
1:B:175:TYR:CE2	1:B:177:MET:HE3	2.00	0.97
1:D:63:VAL:HG12	1:D:95:ARG:NH1	1.79	0.96
1:B:97:ILE:HD11	1:B:177:MET:HE2	1.47	0.95
1:D:66:CRO:HB2	1:D:70:ARG:HH22	1.31	0.95
1:C:65:PHE:C	1:C:66:CRO:N1	2.26	0.93
1:A:66:CRO:C3	1:A:69:ASN:N	2.32	0.93
1:A:224:THR:H	1:B:197:GLN:HE22	1.16	0.93
1:B:171:LYS:NZ	1:B:172:HIS:H	1.66	0.92
1:C:224:THR:H	1:D:197:GLN:HE22	1.13	0.91
1:C:70:ARG:HE	1:C:73:THR:CG2	1.82	0.91
1:C:180:VAL:HB	2:C:324:HOH:O	1.68	0.91
1:C:153:ASN:HA	1:D:171:LYS:HE2	1.51	0.91
1:B:65:PHE:C	1:B:66:CRO:N1	2.29	0.91
1:B:171:LYS:HG3	1:B:172:HIS:N	1.84	0.90
1:A:169:THR:HB	1:C:188:GLU:HG2	1.54	0.90
1:B:66:CRO:C3	1:B:69:ASN:N	2.36	0.89
1:D:65:PHE:C	1:D:66:CRO:N1	2.29	0.89
1:B:85:GLN:HG2	2:B:318:HOH:O	1.73	0.88
1:D:36:ASN:HD22	1:D:39:GLU:H	1.16	0.88
1:C:66:CRO:C3	1:C:69:ASN:N	2.36	0.87
1:C:70:ARG:HE	1:C:73:THR:HG21	1.39	0.86
1:A:54:LEU:HD12	1:A:54:LEU:H	1.40	0.86
1:D:62:SER:O	1:D:66:CRO:N1	2.08	0.85
1:D:66:CRO:C3	1:D:69:ASN:N	2.38	0.85
1:D:98:ARG:HD3	1:D:98:ARG:N	1.91	0.85
1:D:180:VAL:HB	2:D:358:HOH:O	1.77	0.84
1:C:197:GLN:HE22	1:D:224:THR:H	1.26	0.84
1:B:97:ILE:CD1	1:B:177:MET:HE2	2.08	0.83
1:C:63:VAL:HG12	1:C:95:ARG:NH1	1.93	0.83
1:B:70:ARG:O	1:B:73:THR:HG23	1.79	0.83
1:D:66:CRO:HA31	1:D:69:ASN:N	1.94	0.83
1:A:65:PHE:C	1:A:66:CRO:H2	1.82	0.82
1:B:82:TYR:CE1	1:B:187:VAL:HG11	2.14	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:CRO:CA3	1:B:69:ASN:N	2.42	0.82
1:B:171:LYS:HZ2	1:B:172:HIS:H	1.26	0.82
1:C:66:CRO:CA3	1:C:69:ASN:N	2.44	0.81
1:B:188:GLU:H	1:B:188:GLU:CD	1.87	0.81
1:A:10:GLU:HG3	1:A:38:LEU:HD22	1.63	0.81
1:D:66:CRO:CA3	1:D:69:ASN:N	2.44	0.80
1:A:66:CRO:CA3	1:A:69:ASN:N	2.45	0.80
1:B:70:ARG:HE	1:B:73:THR:HG21	1.45	0.80
1:A:70:ARG:HH11	1:A:70:ARG:CG	1.91	0.80
1:A:70:ARG:HG2	1:A:70:ARG:NH1	1.84	0.79
1:A:54:LEU:HD12	1:A:54:LEU:N	1.96	0.79
1:B:189:THR:HG21	1:D:170:GLY:HA3	1.65	0.78
1:A:152:THR:HG22	2:A:251:HOH:O	1.83	0.78
1:A:15:LYS:HG2	1:A:117:LYS:HD2	1.66	0.77
1:D:152:THR:CG2	1:D:190:MET:HB3	2.15	0.77
1:A:70:ARG:O	1:A:73:THR:HG23	1.86	0.76
1:C:89:GLU:OE1	1:C:185:LYS:HD3	1.86	0.75
1:C:193:TYR:CD2	1:D:144:GLN:HG2	2.22	0.75
1:C:66:CRO:HA31	1:C:69:ASN:N	2.02	0.74
1:A:48:VAL:CG2	1:A:54:LEU:HD11	2.17	0.74
1:B:66:CRO:HA31	1:B:69:ASN:N	2.03	0.74
1:B:70:ARG:HE	1:B:73:THR:CG2	2.00	0.74
1:A:171:LYS:HG3	1:A:172:HIS:N	2.02	0.73
1:C:14:THR:HG23	1:C:72:TYR:OH	1.87	0.73
1:D:148:GLU:HA	1:D:161[A]:CYS:HB2	1.69	0.73
1:C:145:PRO:HG3	1:C:199:ARG:HG3	1.71	0.72
1:D:36:ASN:ND2	1:D:39:GLU:H	1.87	0.72
1:A:204:ASN:HB3	1:A:213:VAL:HG12	1.72	0.72
1:A:97:ILE:HG23	1:A:175:TYR:CD2	2.25	0.71
1:D:109:SER:HB2	1:D:122:VAL:HG13	1.70	0.71
1:A:197:GLN:HE22	1:B:224:THR:H	1.38	0.71
1:D:14:THR:HG23	1:D:72:TYR:OH	1.91	0.71
1:B:204:ASN:HB3	1:B:213:VAL:CG1	2.20	0.70
1:B:152[B]:THR:CG2	1:B:191:PRO:HD2	2.21	0.70
1:A:98:ARG:HD2	2:A:263:HOH:O	1.90	0.70
1:D:171:LYS:NZ	1:D:172:HIS:H	1.90	0.70
1:D:114:GLU:H	1:D:116:GLY:HA2	1.57	0.70
1:A:62:SER:HB2	1:A:214:GLN:HE22	1.56	0.69
1:B:204:ASN:HB3	1:B:213:VAL:HG12	1.72	0.69
1:B:152[B]:THR:HG21	1:B:190:MET:HB3	1.75	0.69
1:C:171:LYS:HE2	1:D:153:ASN:HA	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:LYS:HZ2	1:A:50:LYS:HB2	1.58	0.69
1:B:65:PHE:C	1:B:66:CRO:H2	1.97	0.69
1:B:189:THR:HG22	2:C:263:HOH:O	1.92	0.69
1:D:215:HIS:HD2	2:D:257:HOH:O	1.76	0.68
1:C:15:LYS:HG2	1:C:117:LYS:HD2	1.74	0.68
1:A:54:LEU:H	1:A:54:LEU:CD1	2.06	0.68
1:D:70:ARG:HD3	2:D:259:HOH:O	1.92	0.68
1:B:36:ASN:ND2	1:B:38:LEU:H	1.91	0.68
1:B:36:ASN:HD22	1:B:38:LEU:H	1.41	0.68
1:D:109:SER:OG	1:D:122:VAL:HG22	1.92	0.68
1:A:66:CRO:HA31	1:A:69:ASN:N	2.08	0.67
1:B:226:LYS:HB3	2:B:361:HOH:O	1.94	0.67
1:B:15:LYS:NZ	1:B:117:LYS:HD2	2.09	0.67
1:D:141:VAL:HB	1:D:166[A]:LYS:HG3	1.77	0.67
1:B:152[B]:THR:HG22	1:B:191:PRO:HD2	1.76	0.67
1:D:188:GLU:OE1	1:D:189:THR:HG22	1.94	0.67
1:A:62:SER:CB	1:A:214:GLN:HE22	2.08	0.66
1:C:85:GLN:HE21	1:C:187:VAL:CG2	2.09	0.66
1:B:63:VAL:HG12	1:B:95:ARG:NH1	2.10	0.66
1:D:105:ALA:HB1	2:D:350:HOH:O	1.94	0.66
1:B:18:LEU:HD22	1:B:29:MET:HE2	1.76	0.66
1:A:66:CRO:O3	1:A:69:ASN:N	2.28	0.66
1:B:85:GLN:NE2	1:B:187:VAL:HG23	2.11	0.65
1:B:215:HIS:HD2	2:B:250:HOH:O	1.78	0.65
1:C:171:LYS:NZ	1:C:172:HIS:H	1.94	0.65
1:B:100:GLN:NE2	1:B:174:THR:H	1.94	0.65
1:C:204:ASN:HB3	1:C:213:VAL:HG12	1.78	0.65
1:D:100:GLN:HE21	1:D:174:THR:H	1.45	0.65
1:A:50:LYS:HB2	1:A:50:LYS:NZ	2.11	0.65
1:B:98:ARG:HG3	1:B:104:THR:HG22	1.77	0.65
1:C:224:THR:N	1:D:197:GLN:HE22	1.92	0.65
1:A:82:TYR:HE1	1:A:187:VAL:HG11	1.61	0.64
1:D:65:PHE:C	1:D:66:CRO:CA1	2.70	0.64
1:B:148:GLU:HA	1:B:161:CYS:HB3	1.80	0.64
1:A:14:THR:HG23	1:A:72:TYR:OH	1.97	0.64
1:B:177:MET:SD	2:B:379:HOH:O	2.55	0.64
1:C:63:VAL:HG13	1:C:66:CRO:CB2	2.27	0.63
1:C:152:THR:HG22	2:C:343:HOH:O	1.97	0.63
1:D:106:ILE:O	1:D:106:ILE:HG13	1.98	0.63
1:D:152:THR:CG2	1:D:191:PRO:HD2	2.28	0.63
1:D:70:ARG:HG3	1:D:73:THR:HG21	1.78	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:66:CRO:HB2	1:D:70:ARG:NH2	2.11	0.63
1:A:204:ASN:HB3	1:A:213:VAL:CG1	2.29	0.63
1:C:70:ARG:NE	1:C:73:THR:CG2	2.60	0.63
1:D:152:THR:HG22	1:D:191:PRO:HD2	1.80	0.63
1:B:29:MET:HE1	1:B:61:VAL:HG21	1.81	0.63
1:C:153:ASN:CA	1:D:171:LYS:HE2	2.26	0.63
1:B:157:VAL:CG1	1:B:181:TYR:HB2	2.29	0.62
1:B:94:GLU:HG2	2:B:301:HOH:O	1.99	0.62
1:D:114:GLU:N	1:D:116:GLY:HA2	2.11	0.62
1:B:11:VAL:HG22	2:B:285:HOH:O	1.99	0.61
1:D:152:THR:HG21	1:D:190:MET:CB	2.24	0.61
1:C:144:GLN:HG3	1:C:145:PRO:HD2	1.82	0.61
1:B:54:LEU:N	1:B:54:LEU:HD12	2.15	0.60
1:A:14:THR:HG22	1:A:118:PHE:CB	2.14	0.60
1:D:78:GLU:N	1:D:78:GLU:CD	2.59	0.59
1:C:111:ILE:HD12	1:C:111:ILE:N	2.17	0.59
1:A:117:LYS:HE3	1:A:119:ILE:HD11	1.83	0.59
1:A:157:VAL:HG13	1:A:181:TYR:HB2	1.84	0.59
1:B:47:SER:HB2	1:B:211:TYR:HE1	1.68	0.59
1:B:157:VAL:HG13	1:B:181:TYR:HB2	1.84	0.59
1:D:100:GLN:NE2	1:D:174:THR:H	2.00	0.59
1:D:204:ASN:HB3	1:D:213:VAL:HG13	1.83	0.59
1:A:65:PHE:O	1:A:66:CRO:N1	2.36	0.59
1:A:171:LYS:HE2	2:A:361:HOH:O	2.02	0.59
1:C:144:GLN:HG2	1:D:193:TYR:CD2	2.38	0.58
1:A:15:LYS:HE2	1:A:117:LYS:HZ2	1.68	0.58
1:B:15:LYS:HB3	2:B:369:HOH:O	2.02	0.58
1:A:171:LYS:HE3	1:A:172:HIS:O	2.03	0.57
1:D:65:PHE:C	1:D:66:CRO:H2	2.11	0.57
1:D:127:LYS:NZ	1:D:128:ASP:H	2.02	0.57
1:D:171:LYS:HZ3	1:D:172:HIS:H	1.52	0.57
1:B:9:LYS:HG2	2:B:285:HOH:O	2.03	0.57
1:B:171:LYS:CG	1:B:172:HIS:N	2.62	0.57
1:A:63:VAL:HG11	1:A:177:MET:SD	2.44	0.57
1:A:87:PHE:HB3	1:A:88:PRO:HA	1.87	0.57
1:A:180:VAL:HG13	2:A:289:HOH:O	2.04	0.57
1:B:69:ASN:N	2:B:251:HOH:O	2.38	0.57
1:B:63:VAL:HG21	1:B:177:MET:HE1	1.86	0.57
1:C:96:ASN:ND2	1:C:106:ILE:HD12	2.20	0.57
1:D:98:ARG:N	1:D:98:ARG:CD	2.65	0.57
1:C:171:LYS:HE2	1:D:153:ASN:CA	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:148:GLU:HA	1:D:161[B]:CYS:HB3	1.87	0.56
1:C:171:LYS:HE2	1:D:153:ASN:CB	2.35	0.56
2:C:325:HOH:O	1:D:199:ARG:HD2	2.05	0.56
1:C:82:TYR:CE1	1:C:187:VAL:HG11	2.40	0.56
1:D:9:LYS:O	1:D:12:MET:HG2	2.06	0.56
1:B:155:THR:HG22	1:B:155:THR:O	2.05	0.56
1:C:36:ASN:HD22	1:C:38:LEU:H	1.53	0.56
1:C:82:TYR:CD1	1:C:187:VAL:HG11	2.41	0.56
1:B:171:LYS:NZ	1:B:172:HIS:N	2.48	0.56
1:A:151:TYR:HD2	1:B:171:LYS:HZ1	1.55	0.55
1:D:66:CRO:CB2	1:D:70:ARG:HH12	2.20	0.55
1:C:70:ARG:NE	1:C:73:THR:HG21	2.16	0.55
1:C:87:PHE:HB3	1:C:88:PRO:HA	1.89	0.55
1:A:101[B]:ASP:OD2	1:A:130:ARG:HG2	2.07	0.55
1:C:65:PHE:C	1:C:66:CRO:H2	2.11	0.55
1:A:82:TYR:CE1	1:A:187:VAL:HG11	2.41	0.55
1:B:175:TYR:CE2	1:B:177:MET:CE	2.83	0.55
1:D:37:ILE:HG13	1:D:38:LEU:HD13	1.89	0.55
1:A:215:HIS:HD2	2:A:293:HOH:O	1.90	0.54
1:B:70:ARG:NE	1:B:70:ARG:HA	2.21	0.54
1:C:152:THR:CG2	2:C:267:HOH:O	2.54	0.54
1:D:127:LYS:HZ1	1:D:128:ASP:H	1.55	0.54
1:B:15:LYS:HZ2	1:B:117:LYS:HD2	1.71	0.54
1:D:65:PHE:C	1:D:66:CRO:HA1	2.30	0.54
1:B:70:ARG:O	1:B:73:THR:CG2	2.53	0.54
1:C:109:SER:OG	1:C:122:VAL:HG22	2.07	0.54
1:A:105:ALA:HB1	2:A:339:HOH:O	2.07	0.54
1:D:145:PRO:HG3	1:D:199:ARG:HG3	1.89	0.54
1:A:14:THR:HG21	2:A:265:HOH:O	2.08	0.53
1:D:144:GLN:HG3	1:D:145:PRO:HD2	1.90	0.53
1:B:100:GLN:HE21	1:B:174:THR:H	1.56	0.53
1:C:188:GLU:CD	1:C:188:GLU:H	2.14	0.53
1:B:200:LEU:HD23	1:B:200:LEU:C	2.34	0.53
1:A:188:GLU:OE1	1:A:188:GLU:N	2.41	0.53
1:C:70:ARG:HH21	1:C:73:THR:HG22	1.74	0.53
1:A:23:GLY:HA2	1:A:127:LYS:HD2	1.89	0.53
1:A:183:SER:HB3	2:A:337:HOH:O	2.08	0.53
1:C:74:GLY:O	1:C:219:ILE:HD12	2.09	0.53
1:C:94:GLU:HB2	1:C:180:VAL:CG1	2.39	0.53
1:A:169:THR:CB	1:C:188:GLU:HG2	2.33	0.52
1:A:171:LYS:HE3	1:A:172:HIS:H	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:203:THR:OG1	1:C:213:VAL:HG13	2.09	0.52
1:C:144:GLN:HG2	1:D:193:TYR:CG	2.44	0.52
1:C:171:LYS:HE2	1:D:153:ASN:HB2	1.92	0.52
1:B:189:THR:HG23	1:D:169:THR:O	2.10	0.52
1:A:36:ASN:C	1:A:36:ASN:HD22	2.18	0.52
1:C:204:ASN:HB3	1:C:213:VAL:CG1	2.39	0.52
1:C:46:ILE:HD12	1:C:58:PHE:HZ	1.74	0.52
1:A:155:THR:HG22	1:A:155:THR:O	2.09	0.52
1:B:36:ASN:HD22	1:B:36:ASN:C	2.17	0.52
1:B:63:VAL:HG11	1:B:177:MET:SD	2.49	0.52
1:D:15:LYS:HG2	1:D:117:LYS:HD2	1.92	0.52
1:A:77:GLU:CD	1:A:77:GLU:H	2.16	0.52
1:C:66:CRO:O3	1:C:69:ASN:N	2.42	0.52
1:D:154:VAL:HG12	1:D:155:THR:N	2.25	0.52
1:A:28:SER:HB2	1:A:50:LYS:HB2	1.91	0.51
1:B:9:LYS:HD3	2:B:373:HOH:O	2.11	0.51
1:D:63:VAL:HG12	1:D:95:ARG:HH11	1.70	0.51
1:B:70:ARG:HA	1:B:70:ARG:CZ	2.41	0.51
1:C:171:LYS:HZ2	1:C:172:HIS:H	1.58	0.51
1:A:17:ASN:HD22	1:A:121:ASN:HD21	1.58	0.51
1:C:152:THR:HG21	2:C:267:HOH:O	2.10	0.51
1:D:98:ARG:HD3	1:D:98:ARG:H	1.74	0.51
1:B:65:PHE:CA	1:B:66:CRO:N1	2.73	0.51
1:C:36:ASN:HD22	1:C:39:GLU:H	1.57	0.51
1:C:167:LEU:HD12	1:C:171:LYS:HB3	1.92	0.51
1:A:100:GLN:NE2	1:A:174:THR:H	2.08	0.50
1:C:70:ARG:HE	1:C:73:THR:HG22	1.69	0.50
1:D:91:PHE:CZ	1:D:111:ILE:HG13	2.46	0.50
1:A:36:ASN:HD22	1:A:38:LEU:H	1.59	0.50
1:A:152:THR:HG21	2:A:292:HOH:O	2.11	0.50
1:D:63:VAL:HG13	1:D:66:CRO:CB2	2.41	0.50
1:D:202:LYS:HG2	1:D:212:VAL:HG11	1.94	0.50
1:C:66:CRO:HD1	1:C:66:CRO:N2	2.26	0.50
1:D:70:ARG:CD	1:D:73:THR:HG21	2.41	0.50
1:D:97:ILE:HG23	1:D:175:TYR:CD2	2.47	0.50
1:A:155:THR:O	1:A:155:THR:CG2	2.58	0.50
1:B:15:LYS:HZ3	1:B:117:LYS:HD2	1.77	0.50
1:D:109:SER:CB	1:D:122:VAL:HG22	2.42	0.50
1:B:180:VAL:HG11	2:B:306:HOH:O	2.12	0.50
1:B:113:LEU:HD12	1:B:117:LYS:O	2.12	0.50
1:C:11:VAL:HG23	1:C:11:VAL:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:180:VAL:HG11	2:D:288:HOH:O	2.12	0.50
1:B:36:ASN:ND2	1:B:39:GLU:H	2.10	0.49
1:B:85:GLN:NE2	1:B:188:GLU:OE1	2.45	0.49
1:B:171:LYS:HZ2	1:B:172:HIS:N	2.02	0.49
1:D:66:CRO:O3	1:D:69:ASN:N	2.46	0.49
1:D:77:GLU:HB2	1:D:78:GLU:OE2	2.12	0.49
1:A:85:GLN:NE2	1:A:188:GLU:OE1	2.43	0.49
1:A:63:VAL:CG1	1:A:95:ARG:NH1	2.76	0.49
1:C:187:VAL:HG12	2:C:296:HOH:O	2.12	0.49
1:A:171:LYS:CE	1:A:172:HIS:H	2.24	0.49
1:A:188:GLU:CD	1:A:188:GLU:H	2.20	0.49
1:C:219:ILE:HG23	2:C:242:HOH:O	2.12	0.49
1:B:18:LEU:HD22	1:B:29:MET:CE	2.41	0.49
1:D:66:CRO:N2	1:D:66:CRO:HD1	2.28	0.48
1:B:111:ILE:HD12	1:B:111:ILE:N	2.27	0.48
1:A:161[B]:CYS:SG	1:A:177:MET:HE2	2.53	0.48
1:C:109:SER:HG	1:C:122:VAL:HG22	1.78	0.48
1:A:148:GLU:HA	1:A:161[B]:CYS:HB3	1.94	0.48
1:C:36:ASN:ND2	1:C:38:LEU:H	2.11	0.48
1:D:70:ARG:CG	1:D:73:THR:HG21	2.43	0.48
1:B:97:ILE:C	1:B:98:ARG:HD3	2.38	0.48
1:D:87:PHE:HB3	1:D:88:PRO:HA	1.95	0.48
1:D:13:PRO:O	1:D:117:LYS:HG3	2.13	0.48
1:B:175:TYR:HE2	1:B:177:MET:CE	2.03	0.48
1:D:14:THR:CG2	1:D:118:PHE:HB2	2.20	0.48
1:D:171:LYS:HZ2	1:D:172:HIS:H	1.60	0.48
1:B:65:PHE:N	1:B:66:CRO:H2	2.11	0.47
1:B:141:VAL:HB	1:B:166:LYS:HG3	1.96	0.47
1:C:14:THR:CG2	1:C:118:PHE:HB2	2.23	0.47
1:C:144:GLN:HG2	1:D:193:TYR:CE2	2.48	0.47
1:A:157:VAL:CG1	1:A:181:TYR:HB2	2.44	0.47
1:C:37:ILE:HD12	1:C:84:LEU:HD21	1.96	0.47
1:C:171:LYS:HZ3	1:C:172:HIS:H	1.62	0.47
1:D:14:THR:HG21	2:D:263:HOH:O	2.15	0.47
1:D:70:ARG:HD2	1:D:73:THR:HG21	1.95	0.47
1:B:65:PHE:O	1:B:66:CRO:N1	2.47	0.47
1:B:70:ARG:HH21	1:B:73:THR:HG22	1.79	0.47
1:D:29:MET:HB2	1:D:65:PHE:HZ	1.79	0.47
1:D:203:THR:OG1	1:D:213:VAL:HG22	2.15	0.47
1:D:202:LYS:HB2	1:D:202:LYS:HE3	1.70	0.47
1:B:98:ARG:HD3	1:B:98:ARG:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:70:ARG:CZ	1:D:198:HIS:HE1	2.28	0.47
1:A:50:LYS:HE2	2:A:371:HOH:O	2.15	0.46
1:C:65:PHE:C	1:C:66:CRO:CA1	2.88	0.46
1:D:45:LYS:HE3	2:D:285:HOH:O	2.14	0.46
1:C:197:GLN:HE22	1:D:224:THR:N	2.04	0.46
1:B:98:ARG:HB3	2:B:364:HOH:O	2.15	0.46
1:B:203:THR:O	1:B:204:ASN:HB2	2.16	0.46
1:C:36:ASN:ND2	1:C:39:GLU:H	2.14	0.46
1:C:154:VAL:HG12	1:C:155:THR:N	2.30	0.46
1:D:63:VAL:CG1	1:D:95:ARG:NH1	2.67	0.46
1:C:27:PHE:CE2	1:C:56:PHE:CZ	3.03	0.46
1:C:70:ARG:O	1:C:73:THR:HG23	2.16	0.46
1:D:37:ILE:HG13	1:D:38:LEU:CD1	2.46	0.46
1:D:171:LYS:HD2	1:D:171:LYS:HA	1.68	0.46
1:D:127:LYS:HD2	2:D:359:HOH:O	2.16	0.46
1:B:18:LEU:C	1:B:18:LEU:HD23	2.41	0.45
1:B:65:PHE:CA	1:B:66:CRO:H2	2.29	0.45
1:C:114:GLU:HB2	1:C:119:ILE:HG12	1.96	0.45
1:B:27:PHE:HE1	1:B:29:MET:HE2	1.82	0.45
1:B:171:LYS:HG3	1:B:172:HIS:H	1.75	0.45
1:B:152[A]:THR:CG2	2:B:368:HOH:O	2.63	0.45
1:D:54:LEU:HG	1:D:56:PHE:CZ	2.52	0.45
1:C:98:ARG:HG3	2:C:285:HOH:O	2.16	0.45
1:D:148:GLU:HG2	1:D:150:MET:SD	2.56	0.45
1:A:70:ARG:CG	1:A:70:ARG:NH1	2.57	0.45
1:C:97:ILE:HG23	1:C:175:TYR:CD2	2.51	0.45
1:A:15:LYS:NZ	1:A:32:VAL:HG23	2.32	0.45
1:A:65:PHE:CA	1:A:66:CRO:N1	2.78	0.45
1:C:105:ALA:O	1:C:106:ILE:HD13	2.16	0.45
1:B:54:LEU:HD12	1:B:54:LEU:H	1.81	0.45
1:A:189:THR:HG23	1:A:189:THR:O	2.16	0.45
1:B:42:GLN:NE2	1:B:66:CRO:OG1	2.49	0.45
1:B:54:LEU:HA	1:B:55:PRO:HD3	1.70	0.45
1:B:82:TYR:CD1	1:B:187:VAL:HG11	2.50	0.45
1:B:82:TYR:HE1	1:B:187:VAL:HG11	1.75	0.45
1:A:197:GLN:HE22	1:B:224:THR:N	2.12	0.44
1:B:36:ASN:HD22	1:B:38:LEU:N	2.13	0.44
1:B:144:GLN:HB3	1:B:145:PRO:HD2	2.00	0.44
1:C:20:GLY:HA2	1:C:124:PHE:O	2.17	0.44
1:C:152:THR:O	1:D:171:LYS:HE2	2.18	0.44
1:D:12:MET:HE3	1:D:12:MET:HB3	1.87	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:98:ARG:HB2	2:D:312:HOH:O	2.17	0.44
1:A:127:LYS:NZ	1:A:128:ASP:H	2.15	0.44
1:A:144:GLN:HB3	1:A:145:PRO:HD2	1.98	0.44
1:B:66:CRO:HD1	1:B:66:CRO:N2	2.33	0.44
1:B:95:ARG:HB3	1:B:107:VAL:HB	1.99	0.44
1:B:188:GLU:CD	1:B:188:GLU:N	2.64	0.44
1:B:9:LYS:O	1:B:12:MET:HG2	2.18	0.44
1:B:20:GLY:HA2	1:B:124:PHE:O	2.18	0.44
1:C:47:SER:HB2	1:C:211:TYR:CE1	2.52	0.44
1:A:36:ASN:ND2	1:A:39:GLU:H	2.16	0.43
1:B:36:ASN:HD21	1:B:38:LEU:HB2	1.83	0.43
1:B:87:PHE:HB3	1:B:88:PRO:HA	1.99	0.43
1:D:36:ASN:HD21	1:D:38:LEU:HB2	1.83	0.43
1:B:52:ALA:HA	1:B:53:PRO:C	2.42	0.43
1:D:99:TYR:HA	1:D:175:TYR:HB3	1.99	0.43
1:A:65:PHE:CA	1:A:66:CRO:H2	2.32	0.43
1:C:144:GLN:HG2	1:D:193:TYR:CD1	2.53	0.43
1:D:23:GLY:HA2	1:D:127:LYS:HD2	1.99	0.43
1:D:185:LYS:HG3	1:D:186:PRO:HD2	2.00	0.43
1:A:171:LYS:HD2	1:B:153:ASN:OD1	2.19	0.43
1:B:58:PHE:CD2	1:B:58:PHE:C	2.96	0.43
1:D:15:LYS:NZ	1:D:117:LYS:HD2	2.33	0.43
1:B:152[A]:THR:HG22	2:B:242:HOH:O	2.17	0.43
1:B:202:LYS:HE3	1:B:202:LYS:HB2	1.87	0.43
1:D:15:LYS:HZ3	1:D:117:LYS:HD2	1.83	0.43
1:B:180:VAL:HG13	2:B:326:HOH:O	2.18	0.43
1:A:200:LEU:C	1:A:200:LEU:HD23	2.44	0.43
1:B:13:PRO:HD2	1:B:116:GLY:O	2.18	0.43
1:B:43:GLU:O	1:B:43:GLU:HG3	2.17	0.43
1:B:48:VAL:CG2	1:B:54:LEU:HD11	2.30	0.43
1:C:36:ASN:HD22	1:C:36:ASN:C	2.26	0.43
1:A:23:GLY:HA2	1:A:127:LYS:CD	2.48	0.43
1:B:75:TYR:HA	1:B:76:PRO:HD3	1.94	0.43
1:A:22:VAL:HG23	1:A:27:PHE:HE2	1.83	0.42
1:A:212:VAL:HG12	1:A:213:VAL:N	2.34	0.42
1:B:152[B]:THR:HG23	1:B:191:PRO:O	2.18	0.42
1:D:29:MET:HE3	1:D:48:VAL:HG22	2.00	0.42
1:D:16:ILE:HG12	1:D:120:VAL:HB	2.01	0.42
1:D:101:ASP:CG	1:D:173:PHE:HE1	2.26	0.42
1:A:63:VAL:HG12	1:A:95:ARG:NH1	2.35	0.42
1:A:112:SER:HB2	2:A:338:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:158:ILE:HD13	1:C:178:ARG:NH2	2.34	0.42
1:B:82:TYR:CE2	1:B:157:VAL:HG12	2.55	0.42
1:B:130:ARG:HA	1:B:130:ARG:HD2	1.80	0.42
1:B:19:GLU:OE2	1:B:28:SER:OG	2.25	0.42
1:D:152:THR:HG23	1:D:191:PRO:O	2.20	0.42
1:A:24:ASP:N	1:A:24:ASP:OD2	2.52	0.42
1:D:107:VAL:HG22	1:D:124:PHE:CD1	2.55	0.42
1:A:100:GLN:HE21	1:A:174:THR:H	1.68	0.41
1:C:153:ASN:OD1	1:D:171:LYS:HE3	2.20	0.41
1:D:13:PRO:C	1:D:117:LYS:HG3	2.45	0.41
1:A:93:TYR:CE1	1:A:109:SER:HB3	2.56	0.41
1:B:179:THR:HG21	1:B:181:TYR:CZ	2.55	0.41
1:C:75:TYR:HA	1:C:76:PRO:HD3	1.89	0.41
1:A:58:PHE:CE2	1:A:214:GLN:NE2	2.88	0.41
1:C:35:GLY:HA3	1:C:72:TYR:CE2	2.56	0.41
1:D:114:GLU:H	1:D:116:GLY:CA	2.30	0.41
1:D:127:LYS:HZ2	1:D:127:LYS:HA	1.85	0.41
1:A:170:GLY:HA3	1:C:189:THR:OG1	2.20	0.41
1:C:188:GLU:CD	1:C:188:GLU:N	2.79	0.41
1:C:111:ILE:N	1:C:111:ILE:CD1	2.83	0.41
1:D:66:CRO:CA2	1:D:70:ARG:HH12	2.33	0.41
1:A:66:CRO:HD1	1:A:66:CRO:N2	2.36	0.41
1:B:152[A]:THR:HG22	2:B:368:HOH:O	2.21	0.41
1:B:13:PRO:HB2	1:B:117:LYS:HG3	2.03	0.41
1:D:29:MET:CB	1:D:65:PHE:HZ	2.33	0.41
1:B:152[B]:THR:CG2	1:B:190:MET:HB3	2.48	0.41
1:B:171:LYS:CE	1:B:172:HIS:H	2.33	0.41
1:C:65:PHE:N	1:C:66:CRO:H2	2.19	0.41
1:D:106:ILE:HG12	1:D:125:LYS:HB3	2.03	0.40
1:A:179:THR:HG21	1:A:181:TYR:CZ	2.56	0.40
1:C:131:ARG:HG3	2:C:274:HOH:O	2.21	0.40
1:C:149:SER:O	1:C:159:GLY:HA2	2.22	0.40
1:D:117:LYS:HB3	1:D:117:LYS:HE2	1.92	0.40
1:B:44:VAL:O	1:B:213:VAL:HA	2.21	0.40
1:D:70:ARG:CD	1:D:73:THR:CG2	2.99	0.40
1:C:107:VAL:HA	1:C:123:ASP:O	2.21	0.40
1:D:99:TYR:HA	1:D:175:TYR:CB	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	206/239 (86%)	203 (98%)	1 (0%)	2 (1%)	12	2
1	B	210/239 (88%)	205 (98%)	3 (1%)	2 (1%)	12	2
1	C	204/239 (85%)	199 (98%)	4 (2%)	1 (0%)	24	8
1	D	207/239 (87%)	201 (97%)	5 (2%)	1 (0%)	24	8
All	All	827/956 (86%)	808 (98%)	13 (2%)	6 (1%)	18	5

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	154	VAL
1	A	188	GLU
1	B	154	VAL
1	C	154	VAL
1	B	204	ASN
1	D	154	VAL

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	186/206 (90%)	171 (92%)	15 (8%)	11	1
1	B	188/206 (91%)	171 (91%)	17 (9%)	9	0
1	C	184/206 (89%)	170 (92%)	14 (8%)	12	1
1	D	185/206 (90%)	169 (91%)	16 (9%)	10	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	743/824 (90%)	681 (92%)	62 (8%)	11 1

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LEU
1	A	36	ASN
1	A	50	LYS
1	A	54	LEU
1	A	70	ARG
1	A	73	THR
1	A	77	GLU
1	A	127	LYS
1	A	152	THR
1	A	171	LYS
1	A	187	VAL
1	A	188	GLU
1	A	190[A]	MET
1	A	190[B]	MET
1	A	202	LYS
1	B	32	VAL
1	B	36	ASN
1	B	38	LEU
1	B	50	LYS
1	B	54	LEU
1	B	62	SER
1	B	73	THR
1	B	78[A]	GLU
1	B	78[B]	GLU
1	B	84	LEU
1	B	98	ARG
1	B	114	GLU
1	B	171	LYS
1	B	187	VAL
1	B	188	GLU
1	B	202	LYS
1	B	211	TYR
1	C	21	LEU
1	C	36	ASN
1	C	44	VAL
1	C	78	GLU
1	C	98	ARG

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Mol	Chain	Res	Type
1	C	111	ILE
1	C	123	ASP
1	C	127	LYS
1	C	129	LEU
1	C	131	ARG
1	C	152	THR
1	C	188	GLU
1	C	202	LYS
1	C	211	TYR
1	D	21	LEU
1	D	38	LEU
1	D	54	LEU
1	D	84	LEU
1	D	98	ARG
1	D	127	LYS
1	D	129	LEU
1	D	144	GLN
1	D	161[A]	CYS
1	D	161[B]	CYS
1	D	171	LYS
1	D	188	GLU
1	D	202	LYS
1	D	211	TYR
1	D	212	VAL
1	D	213	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	ASN
1	A	42	GLN
1	A	100	GLN
1	A	121	ASN
1	A	138	GLN
1	A	168	GLN
1	A	197	GLN
1	A	214	GLN
1	A	215	HIS
1	B	36	ASN
1	B	42	GLN
1	B	85	GLN
1	B	100	GLN

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Mol	Chain	Res	Type
1	B	138	GLN
1	B	168	GLN
1	B	197	GLN
1	B	215	HIS
1	C	36	ASN
1	C	85	GLN
1	C	96	ASN
1	C	100	GLN
1	C	121	ASN
1	C	138	GLN
1	C	197	GLN
1	D	36	ASN
1	D	42	GLN
1	D	85	GLN
1	D	100	GLN
1	D	138	GLN
1	D	168	GLN
1	D	197	GLN
1	D	214	GLN
1	D	215	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CRO	C	66	-	20,22,24	3.48	4 (20%)	25,30,34	3.47	11 (44%)
1	CRO	D	66	-	20,22,24	3.25	4 (20%)	25,30,34	3.31	10 (40%)
1	CRO	A	66	-	20,22,24	3.58	4 (20%)	25,30,34	3.35	9 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CRO	B	66	-	20,22,24	3.49	5 (25%)	25,30,34	3.34	10 (40%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CRO	C	66	-	-	2/10/29/32	0/2/2/2
1	CRO	D	66	-	-	2/10/29/32	0/2/2/2
1	CRO	A	66	-	-	2/10/29/32	0/2/2/2
1	CRO	B	66	-	-	2/10/29/32	0/2/2/2

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	66	CRO	CB2-CA2	14.47	1.49	1.35
1	C	66	CRO	CB2-CA2	14.21	1.48	1.35
1	B	66	CRO	CB2-CA2	14.17	1.48	1.35
1	D	66	CRO	CB2-CA2	13.13	1.47	1.35
1	A	66	CRO	C1-N2	4.43	1.38	1.32
1	C	66	CRO	C1-N2	3.70	1.37	1.32
1	B	66	CRO	C1-N2	3.62	1.37	1.32
1	C	66	CRO	O2-C2	3.45	1.30	1.23
1	D	66	CRO	C1-N2	3.34	1.37	1.32
1	A	66	CRO	O2-C2	3.25	1.29	1.23
1	D	66	CRO	O2-C2	3.24	1.29	1.23
1	B	66	CRO	O2-C2	2.94	1.29	1.23
1	A	66	CRO	C2-N3	-2.87	1.33	1.40
1	B	66	CRO	C2-N3	-2.75	1.33	1.40
1	D	66	CRO	C2-N3	-2.68	1.33	1.40
1	C	66	CRO	C2-N3	-2.56	1.34	1.40
1	B	66	CRO	CA2-C2	-2.24	1.46	1.48

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	66	CRO	O2-C2-CA2	-12.77	122.87	131.02
1	A	66	CRO	O2-C2-CA2	-11.45	123.71	131.02
1	B	66	CRO	O2-C2-CA2	-11.29	123.81	131.02
1	D	66	CRO	O2-C2-CA2	-10.54	124.30	131.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	66	CRO	CA2-C2-N3	6.37	108.85	103.50
1	D	66	CRO	CB2-CA2-C2	5.82	129.41	122.36
1	B	66	CRO	CA2-C2-N3	5.70	108.29	103.50
1	D	66	CRO	CA2-C2-N3	5.41	108.05	103.50
1	C	66	CRO	CA2-C2-N3	5.29	107.95	103.50
1	D	66	CRO	C2-N3-C1	-5.11	105.70	108.07
1	C	66	CRO	CB2-CA2-C2	5.02	128.44	122.36
1	D	66	CRO	CG2-CB2-CA2	-4.69	124.29	129.87
1	A	66	CRO	C2-N3-C1	-4.41	106.03	108.07
1	B	66	CRO	CB2-CA2-C2	4.38	127.67	122.36
1	B	66	CRO	C2-N3-C1	-4.34	106.06	108.07
1	D	66	CRO	CB2-CA2-N2	-4.18	123.09	128.76
1	C	66	CRO	C2-N3-C1	-4.02	106.21	108.07
1	A	66	CRO	CA1-C1-N3	-4.00	119.63	124.84
1	A	66	CRO	CB2-CA2-C2	3.93	127.12	122.36
1	B	66	CRO	CA3-N3-C2	3.85	132.13	123.67
1	B	66	CRO	CA1-C1-N3	-3.83	119.86	124.84
1	C	66	CRO	CA3-N3-C2	3.82	132.07	123.67
1	A	66	CRO	CA3-N3-C2	3.36	131.04	123.67
1	C	66	CRO	CB2-CA2-N2	-3.25	124.34	128.76
1	A	66	CRO	C2-CA2-N2	-3.03	106.78	108.95
1	C	66	CRO	CG2-CB2-CA2	-3.01	126.29	129.87
1	B	66	CRO	CG2-CB2-CA2	-2.93	126.39	129.87
1	B	66	CRO	C2-CA2-N2	-2.62	107.07	108.95
1	B	66	CRO	CB2-CA2-N2	-2.58	125.25	128.76
1	A	66	CRO	C3-CA3-N3	2.53	118.17	112.43
1	C	66	CRO	C2-CA2-N2	-2.42	107.22	108.95
1	C	66	CRO	O2-C2-N3	2.33	129.18	124.31
1	C	66	CRO	CA1-C1-N3	-2.31	121.83	124.84
1	A	66	CRO	CG2-CB2-CA2	-2.24	127.20	129.87
1	D	66	CRO	CA3-N3-C2	2.15	128.39	123.67
1	C	66	CRO	CD2-CG2-CD1	2.06	120.71	117.65
1	D	66	CRO	CD2-CG2-CB2	-2.03	114.24	121.22
1	D	66	CRO	C2-CA2-N2	-2.03	107.50	108.95
1	D	66	CRO	CD2-CG2-CD1	2.03	120.66	117.65
1	B	66	CRO	CD2-CG2-CD1	2.01	120.63	117.65

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	66	CRO	C3-CA3-N3-C2

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Mol	Chain	Res	Type	Atoms
1	B	66	CRO	C3-CA3-N3-C2
1	C	66	CRO	C3-CA3-N3-C2
1	D	66	CRO	C3-CA3-N3-C2
1	A	66	CRO	C3-CA3-N3-C1
1	B	66	CRO	C3-CA3-N3-C1
1	C	66	CRO	C3-CA3-N3-C1
1	D	66	CRO	C3-CA3-N3-C1

There are no ring outliers.

4 monomers are involved in 46 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	66	CRO	10	0
1	D	66	CRO	15	0
1	A	66	CRO	10	0
1	B	66	CRO	11	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	2
1	B	2
1	C	2
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	66:CRO	C3	69:ASN	N	2.38
1	B	66:CRO	C3	69:ASN	N	2.36
1	C	66:CRO	C3	69:ASN	N	2.36
1	A	66:CRO	C3	69:ASN	N	2.32
1	B	65:PHE	C	66:CRO	N1	2.29
1	D	65:PHE	C	66:CRO	N1	2.29
1	C	65:PHE	C	66:CRO	N1	2.26
1	A	65:PHE	C	66:CRO	N1	2.18

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	211/239 (88%)	1.30	49 (23%) 2 2	8, 22, 39, 72	3 (1%)
1	B	212/239 (88%)	1.51	63 (29%) 1 1	11, 24, 43, 65	4 (1%)
1	C	211/239 (88%)	1.72	87 (41%) 0 0	15, 31, 50, 70	1 (0%)
1	D	211/239 (88%)	2.02	89 (42%) 0 0	14, 35, 58, 82	2 (0%)
All	All	845/956 (88%)	1.64	288 (34%) 1 1	8, 29, 51, 82	10 (1%)

All (288) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	211	TYR	10.9
1	D	211	TYR	10.3
1	D	205	VAL	8.9
1	A	187	VAL	8.0
1	B	211	TYR	7.6
1	B	205	VAL	7.2
1	C	205	VAL	7.0
1	C	211	TYR	6.5
1	A	205	VAL	6.2
1	D	116	GLY	6.0
1	D	11	VAL	5.8
1	A	188	GLU	5.5
1	A	101[A]	ASP	5.1
1	A	114	GLU	5.0
1	D	14	THR	4.9
1	D	114	GLU	4.8
1	B	152[A]	THR	4.7
1	B	101[A]	ASP	4.7
1	D	188	GLU	4.7
1	D	187	VAL	4.7
1	D	7	GLY	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	11	VAL	4.5
1	B	11	VAL	4.5
1	B	187	VAL	4.4
1	D	189	THR	4.4
1	C	48	VAL	4.3
1	D	32	VAL	4.3
1	C	116	GLY	4.2
1	D	9	LYS	4.1
1	C	78	GLU	4.0
1	D	13	PRO	4.0
1	D	88	PRO	4.0
1	B	24	ASP	4.0
1	D	84	LEU	3.9
1	D	15	LYS	3.9
1	B	116	GLY	3.9
1	D	24	ASP	3.9
1	C	180	VAL	3.9
1	C	155	THR	3.8
1	D	106	ILE	3.8
1	D	113	LEU	3.8
1	A	77	GLU	3.8
1	B	226	LYS	3.8
1	C	113	LEU	3.7
1	C	114	GLU	3.7
1	B	213	VAL	3.7
1	D	161[A]	CYS	3.7
1	D	119	ILE	3.7
1	C	85	GLN	3.7
1	D	8	LEU	3.6
1	D	87	PHE	3.6
1	C	24	ASP	3.6
1	D	52	ALA	3.6
1	D	127	LYS	3.5
1	C	106	ILE	3.5
1	A	212	VAL	3.5
1	D	63	VAL	3.5
1	B	169	THR	3.5
1	B	131	ARG	3.5
1	C	39	GLU	3.4
1	B	185	LYS	3.4
1	D	77	GLU	3.4
1	C	187	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	21	LEU	3.4
1	D	38	LEU	3.4
1	A	84	LEU	3.3
1	C	213	VAL	3.3
1	D	122	VAL	3.3
1	A	8	LEU	3.3
1	A	52	ALA	3.3
1	B	157	VAL	3.3
1	A	98	ARG	3.3
1	B	129	LEU	3.2
1	D	180	VAL	3.2
1	B	123	ASP	3.2
1	D	111	ILE	3.2
1	B	48	VAL	3.2
1	D	48	VAL	3.2
1	D	118	PHE	3.2
1	A	15	LYS	3.2
1	C	15	LYS	3.2
1	C	21	LEU	3.1
1	C	38	LEU	3.1
1	C	122	VAL	3.1
1	B	130	ARG	3.1
1	D	193	TYR	3.1
1	B	111	ILE	3.1
1	D	162	ILE	3.1
1	B	115	ASP	3.1
1	A	21	LEU	3.1
1	C	13	PRO	3.1
1	C	125	LYS	3.1
1	B	203	THR	3.0
1	B	154	VAL	3.0
1	D	58	PHE	3.0
1	A	9	LYS	3.0
1	A	226	LYS	3.0
1	D	213	VAL	3.0
1	C	103	GLY	3.0
1	C	14	THR	3.0
1	D	85	GLN	2.9
1	D	226	LYS	2.9
1	C	56	PHE	2.9
1	D	91	PHE	2.9
1	D	33	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	168	GLN	2.9
1	B	73	THR	2.9
1	C	26	ALA	2.9
1	C	185	LYS	2.9
1	A	88	PRO	2.9
1	A	70	ARG	2.9
1	A	189	THR	2.9
1	D	44	VAL	2.9
1	B	77[A]	GLU	2.9
1	A	24	ASP	2.8
1	C	111	ILE	2.8
1	D	37	ILE	2.8
1	C	77	GLU	2.8
1	A	14	THR	2.8
1	C	28	SER	2.8
1	B	22	VAL	2.8
1	C	188	GLU	2.8
1	C	124	PHE	2.8
1	C	9	LYS	2.8
1	B	183	SER	2.8
1	A	7	GLY	2.8
1	B	186	PRO	2.8
1	D	53	PRO	2.8
1	D	132	MET	2.8
1	C	184	LYS	2.8
1	D	74	GLY	2.8
1	A	131	ARG	2.8
1	B	44	VAL	2.7
1	C	168	GLN	2.7
1	C	186	PRO	2.7
1	B	54	LEU	2.7
1	D	101	ASP	2.7
1	D	154	VAL	2.7
1	D	201	VAL	2.7
1	C	7	GLY	2.7
1	C	131	ARG	2.7
1	B	125	LYS	2.7
1	C	50	LYS	2.7
1	D	86	SER	2.7
1	C	64	ALA	2.7
1	D	70	ARG	2.7
1	B	122	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	214	GLN	2.7
1	C	119	ILE	2.7
1	D	93	TYR	2.6
1	A	38	LEU	2.6
1	B	114	GLU	2.6
1	C	135	VAL	2.6
1	C	212	VAL	2.6
1	C	45	LYS	2.6
1	D	110	ASP	2.6
1	A	190[A]	MET	2.6
1	B	212	VAL	2.6
1	D	144	GLN	2.6
1	C	123	ASP	2.6
1	C	161	CYS	2.6
1	B	155	THR	2.6
1	B	84	LEU	2.6
1	C	204	ASN	2.6
1	A	201	VAL	2.6
1	C	44	VAL	2.6
1	C	169	THR	2.5
1	D	47	SER	2.5
1	D	89	GLU	2.5
1	B	168	GLN	2.5
1	B	98	ARG	2.5
1	D	131	ARG	2.5
1	C	84	LEU	2.5
1	B	55	PRO	2.5
1	A	48	VAL	2.5
1	B	63	VAL	2.5
1	A	204	ASN	2.5
1	C	130	ARG	2.5
1	B	188	GLU	2.5
1	D	94	GLU	2.5
1	B	124	PHE	2.5
1	C	127	LYS	2.5
1	C	171	LYS	2.5
1	D	117	LYS	2.5
1	A	186	PRO	2.4
1	C	65	PHE	2.4
1	C	94	GLU	2.4
1	C	170	GLY	2.4
1	D	23	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	101[A]	ASP	2.4
1	D	25	HIS	2.4
1	A	87	PHE	2.4
1	A	157	VAL	2.4
1	C	63	VAL	2.4
1	C	88	PRO	2.4
1	D	186	PRO	2.4
1	B	21	LEU	2.4
1	C	54	LEU	2.4
1	C	58	PHE	2.4
1	C	118	PHE	2.4
1	D	153	ASN	2.4
1	D	107	VAL	2.3
1	D	212	VAL	2.3
1	A	53	PRO	2.3
1	C	49	THR	2.3
1	D	46	ILE	2.3
1	B	91	PHE	2.3
1	A	44	VAL	2.3
1	A	135	VAL	2.3
1	A	155	THR	2.3
1	C	203	THR	2.3
1	C	20	GLY	2.3
1	C	79	ILE	2.3
1	A	57	ALA	2.3
1	B	30	GLU	2.3
1	D	112	SER	2.3
1	B	56	PHE	2.3
1	C	87	PHE	2.3
1	B	204	ASN	2.3
1	C	61	VAL	2.3
1	C	73	THR	2.3
1	D	73	THR	2.3
1	D	168	GLN	2.3
1	A	50	LYS	2.3
1	D	225	ILE	2.3
1	D	152	THR	2.2
1	B	141	VAL	2.2
1	C	11	VAL	2.2
1	A	127	LYS	2.2
1	C	202	LYS	2.2
1	C	52	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	26	ALA	2.2
1	C	53	PRO	2.2
1	D	92	THR	2.2
1	D	203	THR	2.2
1	D	90	GLY	2.2
1	C	27	PHE	2.2
1	D	183	SER	2.2
1	C	154	VAL	2.2
1	C	8	LEU	2.2
1	C	167	LEU	2.2
1	B	39	GLU	2.2
1	B	94	GLU	2.2
1	C	89	GLU	2.2
1	D	140	ILE	2.2
1	B	53	PRO	2.2
1	B	117	LYS	2.2
1	C	138	GLN	2.2
1	D	65	PHE	2.2
1	B	32	VAL	2.2
1	B	50	LYS	2.2
1	D	185	LYS	2.2
1	B	113	LEU	2.1
1	D	54	LEU	2.1
1	C	57	ALA	2.1
1	D	76	PRO	2.1
1	C	46	ILE	2.1
1	C	41	THR	2.1
1	A	39	GLU	2.1
1	A	56	PHE	2.1
1	C	120	VAL	2.1
1	B	13	PRO	2.1
1	B	51	GLY	2.1
1	D	51	GLY	2.1
1	A	203	THR	2.1
1	C	16	ILE	2.1
1	C	226	LYS	2.1
1	A	116	GLY	2.1
1	D	56	PHE	2.1
1	B	49	THR	2.1
1	B	38	LEU	2.1
1	D	167	LEU	2.1
1	B	15	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	181	TYR	2.1
1	B	78[A]	GLU	2.1
1	C	55	PRO	2.1
1	A	65	PHE	2.0
1	B	9	LYS	2.0
1	B	178	ARG	2.0
1	D	10	GLU	2.0
1	D	43	GLU	2.0
1	D	75	TYR	2.0
1	C	110	ASP	2.0
1	A	171	LYS	2.0
1	B	171	LYS	2.0
1	A	49	THR	2.0
1	D	49	THR	2.0
1	A	213	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	CRO	B	66	21/23	0.91	0.12	11,20,30,34	0
1	CRO	D	66	21/23	0.91	0.12	26,31,37,40	0
1	CRO	C	66	21/23	0.92	0.12	26,30,35,40	0
1	CRO	A	66	21/23	0.93	0.10	12,16,20,32	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.