Full wwPDB X-ray Structure Validation Report (i)

Oct 17, 2026 – 10:21 am BST

PDB ID	:	9QE8 / pdb_00009qe8
Title	:	SMAD4 MH2 domain (residues 314-552) bound by Nanobody A7 (NbA7)
Authors	:	Pluta, R.; Macias, M.J.; Condeminas, M.
Deposited on	:	2025-03-07
Resolution	:	3.04 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 (i) 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 (1)) were used in the production of this report:

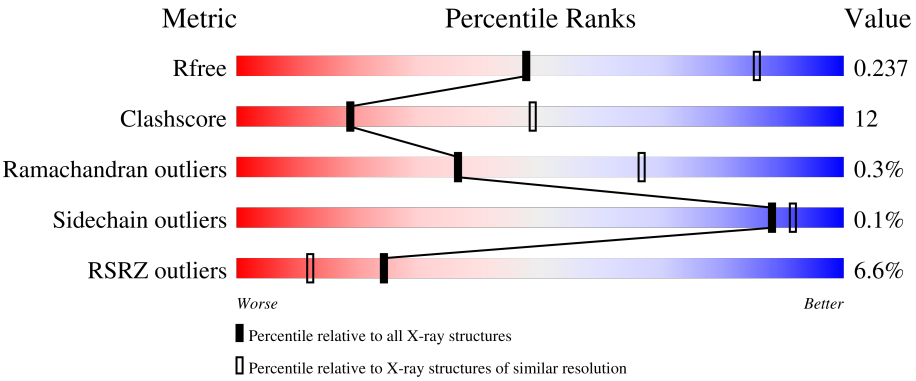
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.04 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	3685 (3.08-3.00)
Clashscore	190562	4007 (3.08-3.00)
Ramachandran outliers	187476	3834 (3.08-3.00)
Sidechain outliers	187428	3836 (3.08-3.00)
RSRZ outliers	180081	3684 (3.08-3.00)

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 <=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	240	% 66% 12% 21%
1	C	240	3% 59% 19% 22%
1	E	240	2% 56% 19% 25%
1	G	240	5% 63% 16% 21%
1	I	240	2% 59% 19% 22%

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Mol	Chain	Length	Quality of chain
1	K	240	2% 62% 15% 22%
2	B	126	5% 60% 29% 10%
2	D	126	10% 55% 33% 12%
2	F	126	6% 59% 30% 11%
2	H	126	10% 66% 24% 10%
2	J	126	10% 61% 24% 15%
2	L	126	23% 52% 25% 22%

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
3	ACT	C	602	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 27470 atoms, of which 13456 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 Mothers against decapentaplegic homolog 4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	189	Total	C	H	N	O	S	0	0	0
			2982	956	1470	271	274	11			
1	C	187	Total	C	H	N	O	S	0	0	0
			2957	948	1459	268	271	11			
1	E	181	Total	C	H	N	O	S	0	0	0
			2862	922	1408	259	262	11			
1	G	190	Total	C	H	N	O	S	0	0	0
			3000	961	1481	272	275	11			
1	I	188	Total	C	H	N	O	S	0	0	0
			2964	951	1461	269	272	11			
1	K	187	Total	C	H	N	O	S	0	0	0
			2921	942	1435	262	271	11			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	313	GLY	-	expression tag	UNP Q13485
C	313	GLY	-	expression tag	UNP Q13485
E	313	GLY	-	expression tag	UNP Q13485
G	313	GLY	-	expression tag	UNP Q13485
I	313	GLY	-	expression tag	UNP Q13485
K	313	GLY	-	expression tag	UNP Q13485

- Molecule 2 is a protein called Nanobody A7 (NbA7).

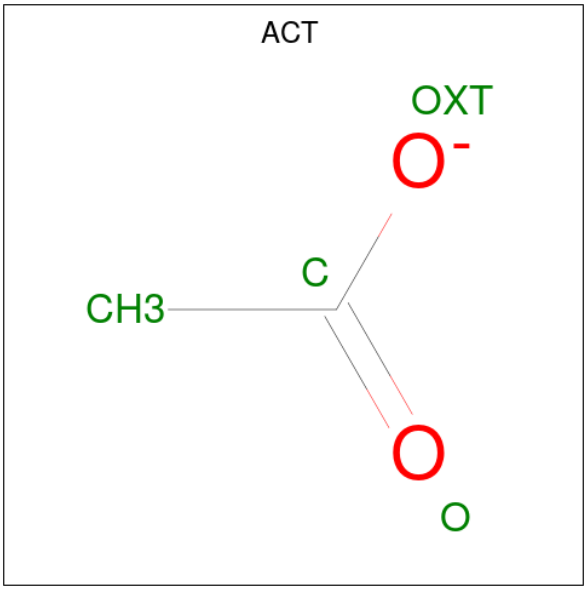
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	113	Total	C	H	N	O	S	0	0	0
			1668	536	811	147	170	4			
2	D	111	Total	C	H	N	O	S	0	0	0
			1651	531	805	147	164	4			
2	F	112	Total	C	H	N	O	S	0	0	0
			1647	530	797	146	170	4			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	H	113	Total	C	H	N	O	S	0	0	0
			1655	534	801	146	170	4			
2	J	107	Total	C	H	N	O	S	0	0	0
			1586	509	768	143	162	4			
2	L	98	Total	C	H	N	O	S	0	0	0
			1365	454	647	119	141	4			

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



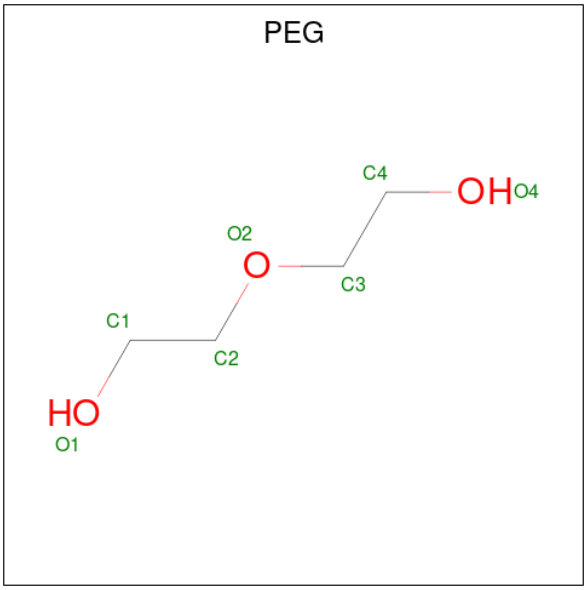
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			7	2	3	2		
3	A	1	Total	C	H	O	0	0
			7	2	3	2		
3	C	1	Total	C	H	O	0	0
			7	2	3	2		
3	C	1	Total	C	H	O	0	0
			7	2	3	2		
3	C	1	Total	C	H	O	0	0
			7	2	3	2		
3	D	1	Total	C	H	O	0	0
			7	2	3	2		
3	E	1	Total	C	H	O	0	0
			7	2	3	2		
3	F	1	Total	C	H	O	0	0
			7	2	3	2		

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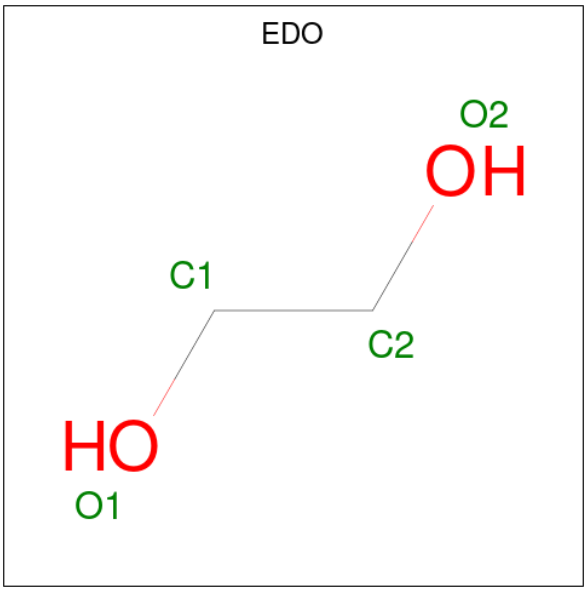
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	F	1	Total C H O 7 2 3 2	0	0
3	I	1	Total C H O 7 2 3 2	0	0
3	J	1	Total C H O 7 2 3 2	0	0

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C H O 17 4 10 3	0	0
4	F	1	Total C H O 17 4 10 3	0	0
4	G	1	Total C H O 17 4 10 3	0	0
4	H	1	Total C H O 17 4 10 3	0	0
4	I	1	Total C H O 17 4 10 3	0	0

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



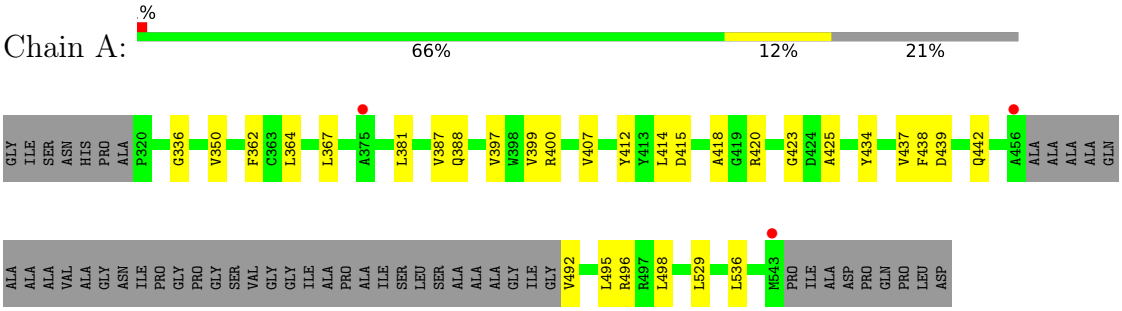
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	C	1	Total	C	H	O	0	0
			10	2	6	2		
5	E	1	Total	C	H	O	0	0
			10	2	6	2		
5	G	1	Total	C	H	O	0	0
			10	2	6	2		
5	K	1	Total	C	H	O	0	0
			10	2	6	2		

3 Residue-property plots (i)

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.

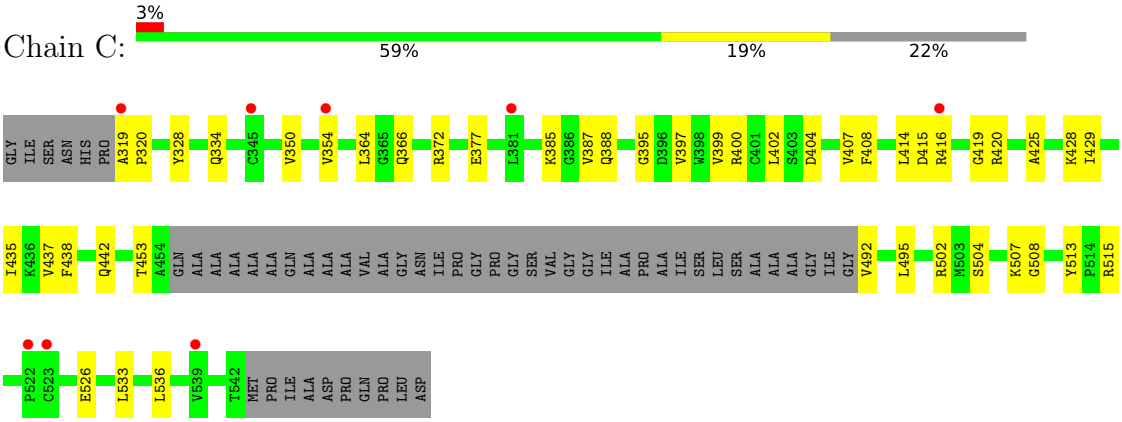
• Molecule 1: Mothers against decapentaplegic homolog 4

Chain A:



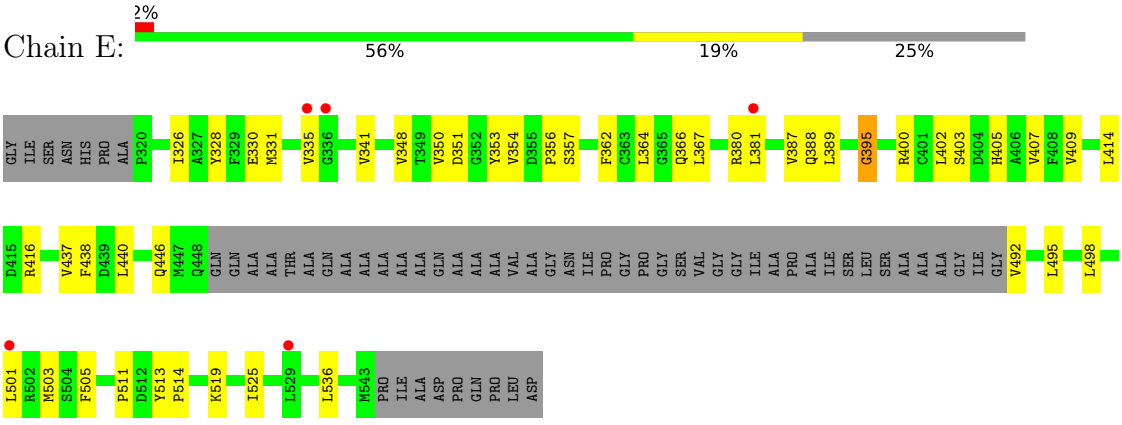
• Molecule 1: Mothers against decapentaplegic homolog 4

Chain C:



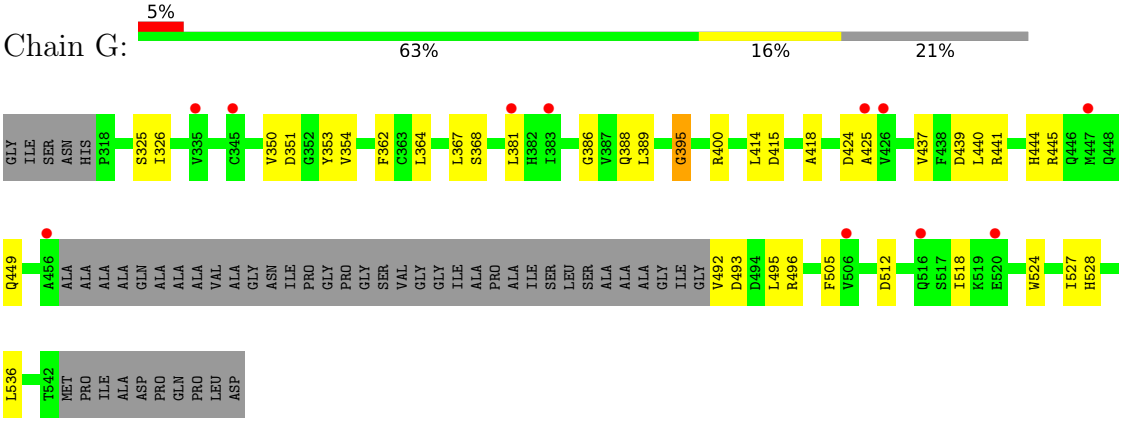
• Molecule 1: Mothers against decapentaplegic homolog 4

Chain E:



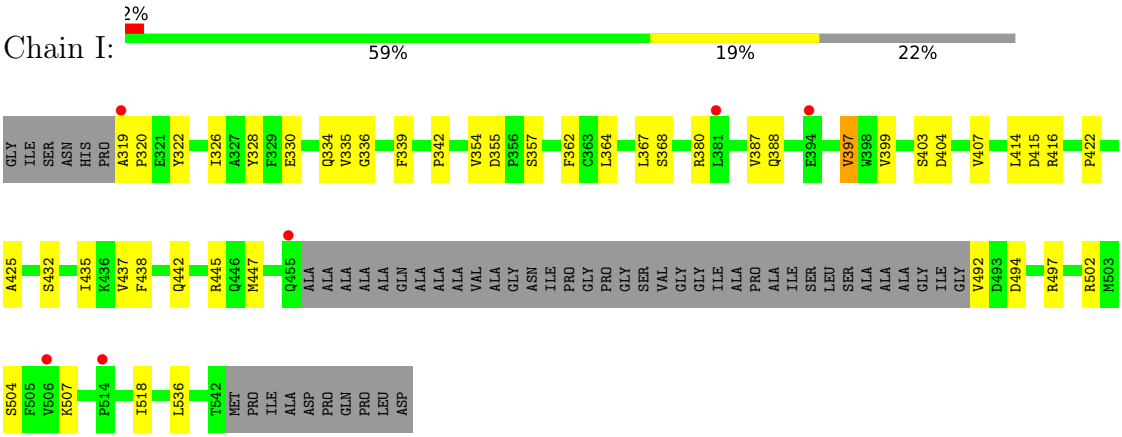
• Molecule 1: Mothers against decapentaplegic homolog 4

Chain G:



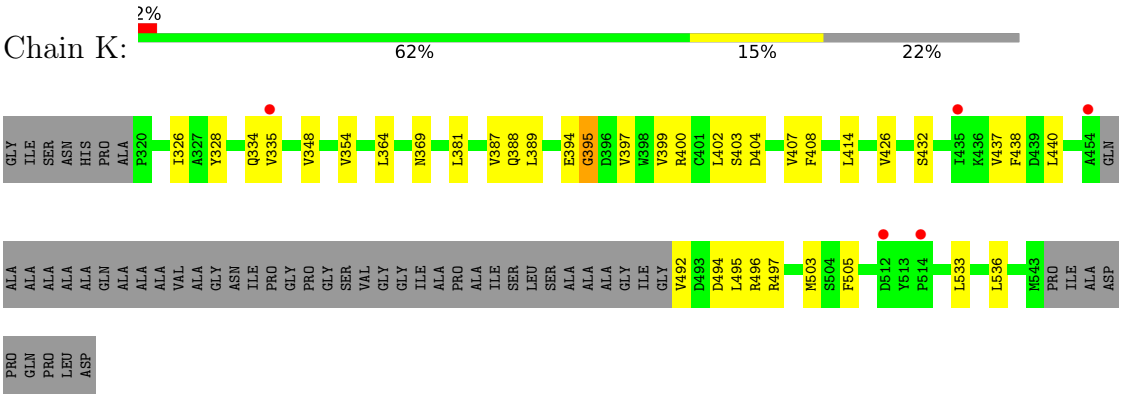
• Molecule 1: Mothers against decapentaplegic homolog 4

Chain I:



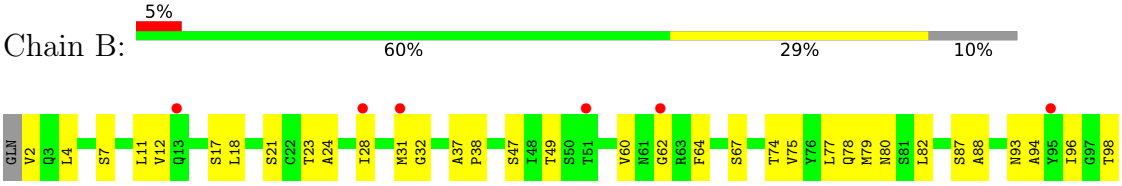
• Molecule 1: Mothers against decapentaplegic homolog 4

Chain K:



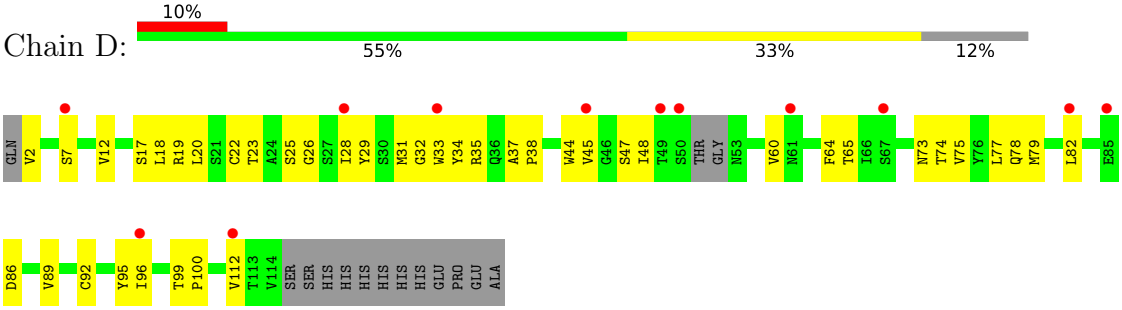
• Molecule 2: Nanobody A7 (NbA7)

Chain B:

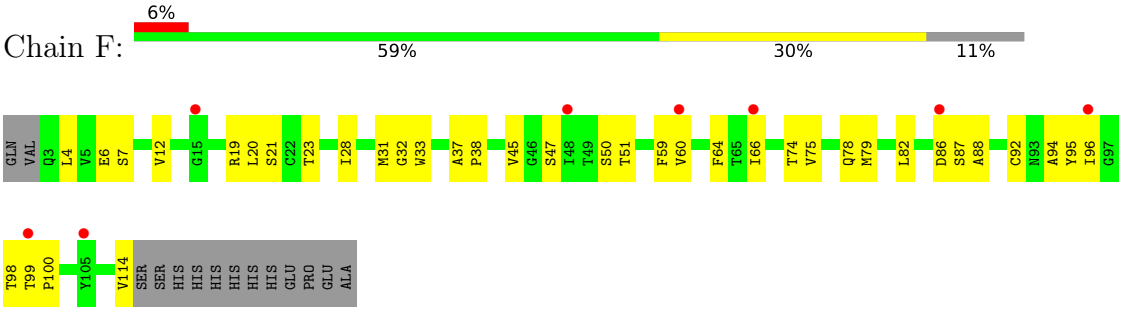




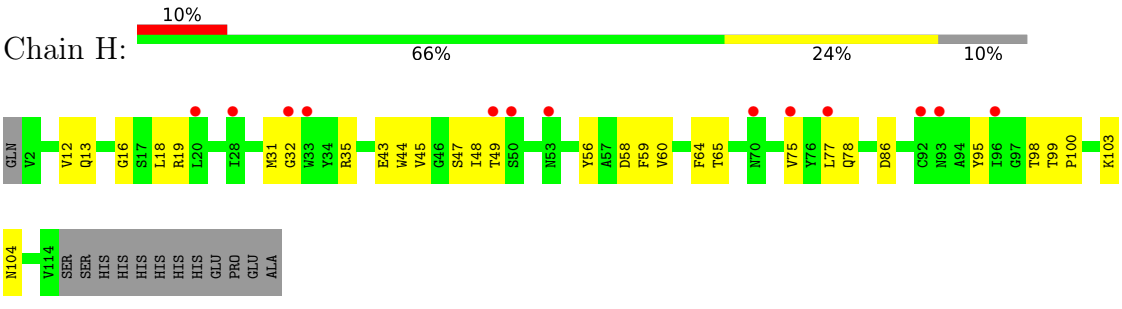
• Molecule 2: Nanobody A7 (NbA7)



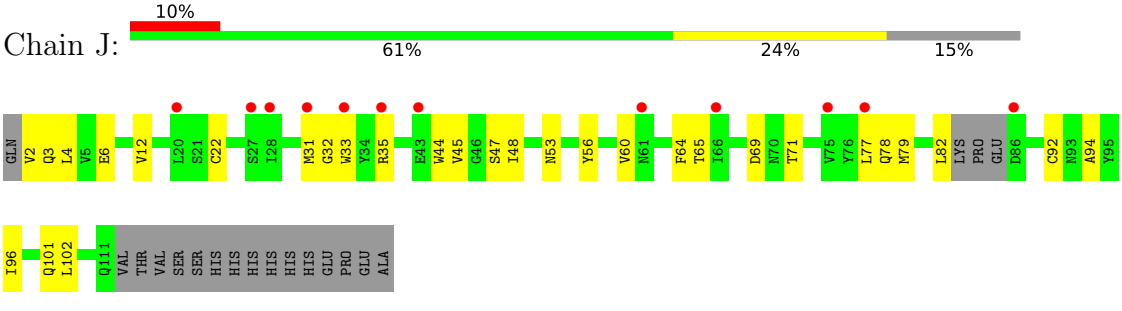
• Molecule 2: Nanobody A7 (NbA7)



• Molecule 2: Nanobody A7 (NbA7)

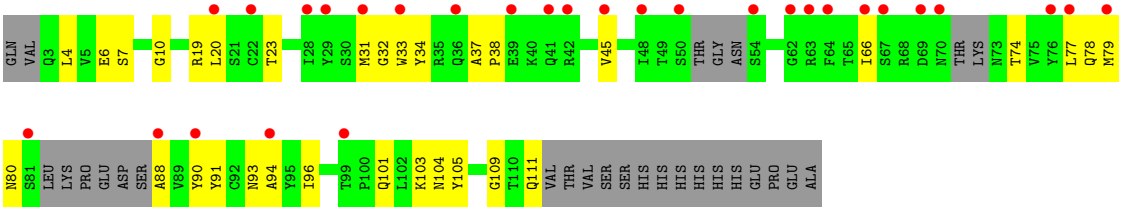


• Molecule 2: Nanobody A7 (NbA7)



• Molecule 2: Nanobody A7 (NbA7)




GLN VAL Q3 L4 V5 E6 S7 G10 R19 L20 S21 C22 T23 I28 Y29 S30 M31 G32 W33 Y34 R35 Q36 A37 P38 E39 K40 Q41 R42 V45 I48 T49 S50 THR GLY ASN S54 G62 R63 F64 T65 I66 S67 R68 D69 N70 THR LYS N73 T74 V75 Y76 L77 Q78 M79
N80 S81 LEU LYS PRO GLU ASP SER A88 V89 Y90 Y91 C92 N93 A94 Y95 I96 T99 P100 Q101 L102 K103 N104 Y105 G109 T110 Q111 VAL THR VAL SER SER HIS HIS HIS HIS HIS HIS GLU PRO GLU ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	42.13Å 147.90Å 148.86Å 119.93° 94.33° 89.31°	Depositor
Resolution (Å)	74.22 – 3.04 74.22 – 3.04	Depositor EDS
% Data completeness (in resolution range)	47.0 (74.22-3.04) 47.0 (74.22-3.04)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.59 (at 3.07Å)	Xtriage
Refinement program	PHENIX 1.21rc1_5107	Depositor
R, R_{free}	0.227 , 0.274 0.230 , 0.237	Depositor DCC
R_{free} test set	1332 reflections (2.23%)	wwPDB-VP
Wilson B-factor (Å^2)	36.9	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 48.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.048 for -h,k,-k-l	Xtriage
F_o,F_c correlation	0.83	EDS
Total number of atoms	27470	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.08% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: EDO, ACT, PEG

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	0.16	0/1549	0.41	0/2098
1	C	0.17	0/1535	0.45	0/2080
1	E	0.15	0/1491	0.37	0/2020
1	G	0.17	0/1557	0.43	0/2110
1	I	0.16	0/1540	0.41	0/2087
1	K	0.16	0/1523	0.44	0/2065
2	B	0.20	0/875	0.45	0/1190
2	D	0.20	0/863	0.44	0/1171
2	F	0.20	0/868	0.49	0/1181
2	H	0.20	0/872	0.48	0/1187
2	J	0.20	0/834	0.45	0/1131
2	L	0.17	0/732	0.46	0/994
All	All	0.17	0/14239	0.44	0/19314

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1512	1470	1470	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1498	1459	1459	38	0
1	E	1454	1408	1408	36	0
1	G	1519	1481	1480	26	0
1	I	1503	1461	1461	34	1
1	K	1486	1435	1435	27	1
2	B	857	811	811	33	1
2	D	846	805	805	33	1
2	F	850	797	797	26	0
2	H	854	801	802	27	1
2	J	818	768	767	23	0
2	L	718	647	643	24	0
3	A	8	6	6	0	0
3	C	12	9	9	5	0
3	D	4	3	3	0	0
3	E	4	3	3	0	0
3	F	8	6	6	0	0
3	I	4	3	3	0	0
3	J	4	3	3	0	0
4	A	7	10	10	0	0
4	F	7	10	10	0	0
4	G	7	10	10	0	0
4	H	7	10	10	0	1
4	I	7	10	10	2	0
5	A	4	6	6	0	0
5	C	4	6	6	0	0
5	E	4	6	6	0	0
5	G	4	6	6	1	0
5	K	4	6	6	0	0
All	All	14014	13456	13451	328	3

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 12.

All (328) 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:C:416:ARG:NH1	1:C:442:GLN:OE1	2.04	0.89
1:I:494:ASP:OD1	1:I:497:ARG:NH1	2.06	0.88
2:H:31:MET:HE2	2:H:75:VAL:HG11	1.56	0.86
1:C:504:SER:OG	1:C:507:LYS:O	1.98	0.82
1:C:492:VAL:HA	1:C:495:LEU:HD23	1.60	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:387:VAL:HG11	1:I:407:VAL:HG21	1.63	0.79
2:D:35:ARG:NH1	2:D:86:ASP:OD1	2.17	0.77
1:E:492:VAL:HA	1:E:495:LEU:HD23	1.67	0.77
1:I:536:LEU:HD22	1:K:354:VAL:HG21	1.69	0.74
2:J:22:CYS:HB3	2:J:31:MET:HE1	1.69	0.73
1:C:415:ASP:OD1	1:C:425:ALA:HB3	1.89	0.73
1:E:387:VAL:HG11	1:E:407:VAL:HG21	1.71	0.72
2:D:31:MET:HE2	2:D:75:VAL:HB	1.72	0.71
1:E:387:VAL:CG1	1:E:407:VAL:HG21	2.21	0.70
2:L:66:ILE:HG23	2:L:77:LEU:HD13	1.73	0.70
2:B:23:THR:HG23	2:B:74:THR:CG2	2.22	0.69
2:H:60:VAL:HG21	2:H:64:PHE:HB2	1.76	0.68
2:J:48:ILE:HG13	2:J:53:ASN:O	1.94	0.67
2:L:66:ILE:CG2	2:L:77:LEU:HD13	2.24	0.66
2:B:60:VAL:HG23	2:B:60:VAL:O	1.95	0.66
2:D:22:CYS:HB3	2:D:31:MET:HE1	1.78	0.66
1:I:397:VAL:HG12	1:I:438:PHE:HB3	1.78	0.66
2:F:31:MET:HG2	2:F:32:GLY:N	2.10	0.65
1:A:387:VAL:HG11	1:A:407:VAL:HG21	1.79	0.65
2:H:64:PHE:HB3	2:H:77:LEU:HD11	1.79	0.64
2:J:2:VAL:CG1	2:J:96:ILE:HD11	2.28	0.64
2:H:12:VAL:HG21	2:H:18:LEU:HG	1.80	0.63
2:H:19:ARG:NH1	2:H:78:GLN:OE1	2.31	0.63
1:K:495:LEU:HB3	1:K:536:LEU:HD11	1.81	0.62
2:B:12:VAL:HG11	2:B:82:LEU:HD12	1.81	0.62
1:A:418:ALA:HA	2:B:49:THR:HG22	1.80	0.62
2:H:31:MET:SD	2:H:32:GLY:N	2.72	0.62
2:H:35:ARG:NE	2:H:43:GLU:OE1	2.28	0.62
1:I:536:LEU:HD23	1:I:536:LEU:O	2.00	0.62
2:J:4:LEU:HD11	2:J:94:ALA:HB3	1.81	0.62
2:F:79:MET:HB3	2:F:82:LEU:HD21	1.81	0.62
1:A:536:LEU:HD23	1:C:354:VAL:HG21	1.82	0.62
1:C:508:GLY:H	3:C:602:ACT:H1	1.64	0.61
1:I:415:ASP:OD1	1:I:425:ALA:HB3	2.00	0.61
2:B:18:LEU:HD12	2:B:112:VAL:HG13	1.83	0.61
2:B:23:THR:HG23	2:B:74:THR:HG22	1.80	0.61
2:B:98:THR:HB	2:B:100:PRO:HD2	1.81	0.61
2:J:31:MET:HG2	2:J:32:GLY:N	2.15	0.61
2:F:19:ARG:NH1	2:F:78:GLN:OE1	2.33	0.61
1:K:492:VAL:HA	1:K:495:LEU:HD23	1.83	0.61
1:I:504:SER:OG	1:I:507:LYS:O	2.10	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:416:ARG:CZ	2:J:102:LEU:HD12	2.31	0.60
2:J:56:TYR:HB3	2:J:60:VAL:HG21	1.81	0.60
2:L:37:ALA:HB2	2:L:88:ALA:HB2	1.83	0.60
1:A:495:LEU:HB3	1:A:536:LEU:HD11	1.83	0.60
1:G:354:VAL:HB	1:K:533:LEU:HD22	1.83	0.59
2:D:2:VAL:HG13	2:D:25:SER:HB3	1.83	0.59
1:C:515:ARG:NH1	3:C:602:ACT:H2	2.17	0.59
2:F:31:MET:O	2:F:47:SER:HB2	2.02	0.59
2:H:98:THR:HB	2:H:100:PRO:HD2	1.84	0.59
2:F:4:LEU:HD11	2:F:94:ALA:HB3	1.83	0.59
1:K:394:GLU:N	1:K:394:GLU:OE1	2.35	0.59
1:I:319:ALA:HB3	1:I:320:PRO:HD3	1.83	0.59
1:K:395:GLY:HA3	1:K:440:LEU:HD22	1.83	0.59
2:J:69:ASP:O	2:J:71:THR:N	2.33	0.59
1:E:328:TYR:OH	1:E:330:GLU:OE2	2.14	0.59
2:D:18:LEU:HD12	2:D:112:VAL:HG13	1.85	0.58
1:E:330:GLU:OE2	1:E:380:ARG:HD2	2.03	0.58
1:G:415:ASP:OD1	1:G:425:ALA:HB3	2.04	0.58
2:D:60:VAL:HG21	2:D:64:PHE:HB2	1.86	0.58
1:G:414:LEU:HD11	1:G:437:VAL:HG12	1.86	0.58
2:J:33:TRP:O	2:J:45:VAL:HG22	2.03	0.58
2:B:31:MET:HG2	2:B:32:GLY:N	2.19	0.57
1:E:492:VAL:CA	1:E:495:LEU:HD23	2.34	0.57
2:J:35:ARG:HD3	2:J:45:VAL:HG11	1.84	0.57
2:J:79:MET:HB3	2:J:82:LEU:HD21	1.86	0.57
1:I:328:TYR:CE1	1:I:364:LEU:HD13	2.39	0.57
1:A:387:VAL:CG1	1:A:407:VAL:HG21	2.35	0.57
1:C:513:TYR:HD2	3:C:602:ACT:H3	1.68	0.57
2:B:31:MET:SD	2:B:75:VAL:HB	2.44	0.56
2:L:104:ASN:OD1	2:L:105:TYR:N	2.37	0.56
1:C:414:LEU:HD11	1:C:437:VAL:HG12	1.87	0.56
2:D:12:VAL:HG11	2:D:82:LEU:HD12	1.88	0.56
2:F:33:TRP:HD1	2:F:66:ILE:HD12	1.70	0.56
1:E:350:VAL:CG1	1:E:364:LEU:HD11	2.36	0.56
2:F:31:MET:SD	2:F:75:VAL:HG11	2.46	0.56
1:K:494:ASP:OD1	1:K:497:ARG:NH1	2.39	0.55
1:A:492:VAL:HA	1:A:495:LEU:HD23	1.89	0.55
1:I:435:ILE:HG23	1:I:437:VAL:HG13	1.89	0.54
1:I:502:ARG:HB3	1:I:518:ILE:HD13	1.89	0.54
1:I:403:SER:OG	1:I:404:ASP:N	2.40	0.54
2:J:56:TYR:HB3	2:J:60:VAL:CG2	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:33:TRP:O	2:L:45:VAL:HG22	2.07	0.54
1:E:438:PHE:HB2	1:E:501:LEU:HD11	1.90	0.54
2:H:31:MET:HE2	2:H:75:VAL:CG1	2.34	0.54
1:C:515:ARG:HH12	3:C:602:ACT:H2	1.74	0.53
2:H:31:MET:CE	2:H:75:VAL:HG11	2.34	0.53
2:J:64:PHE:HB3	2:J:77:LEU:HD11	1.90	0.53
2:B:11:LEU:HD23	2:B:12:VAL:N	2.24	0.53
1:E:513:TYR:HB3	1:E:514:PRO:HD2	1.90	0.53
1:E:328:TYR:HA	1:E:525:ILE:HG22	1.91	0.52
2:F:98:THR:HB	2:F:100:PRO:HD2	1.90	0.52
1:K:388:GLN:HG3	1:K:402:LEU:HD12	1.91	0.52
2:D:22:CYS:CB	2:D:31:MET:HE1	2.40	0.52
1:E:387:VAL:HG21	1:E:503:MET:SD	2.50	0.52
2:B:7:SER:O	2:B:21:SER:N	2.40	0.52
1:A:336:GLY:HA3	1:A:367:LEU:HD13	1.90	0.52
2:J:12:VAL:HG11	2:J:82:LEU:HD12	1.92	0.52
1:C:387:VAL:HG11	1:C:407:VAL:HG21	1.91	0.51
2:L:78:GLN:HG3	2:L:80:ASN:HD21	1.75	0.51
1:C:492:VAL:HG12	1:E:381:LEU:HD11	1.92	0.51
1:C:319:ALA:HB3	1:C:320:PRO:HD3	1.92	0.51
2:D:23:THR:HG23	2:D:74:THR:HG22	1.92	0.51
2:L:6:GLU:OE1	2:L:6:GLU:N	2.42	0.51
2:F:7:SER:O	2:F:20:LEU:HA	2.09	0.51
1:I:414:LEU:HD11	1:I:437:VAL:HG12	1.92	0.51
2:D:35:ARG:HA	2:D:89:VAL:O	2.11	0.51
1:K:414:LEU:HD11	1:K:437:VAL:HG12	1.93	0.51
1:E:395:GLY:HA3	1:E:440:LEU:HD22	1.93	0.51
1:G:518:ILE:HD11	1:G:524:TRP:HB2	1.92	0.51
2:L:96:ILE:O	2:L:103:LYS:HG2	2.11	0.50
2:F:45:VAL:HG12	2:F:45:VAL:O	2.10	0.50
2:B:31:MET:HA	2:B:93:ASN:O	2.11	0.50
1:K:403:SER:OG	1:K:404:ASP:N	2.45	0.50
1:C:399:VAL:HG23	1:C:437:VAL:HG21	1.94	0.50
2:D:19:ARG:HA	2:D:77:LEU:O	2.12	0.50
2:F:7:SER:O	2:F:21:SER:N	2.45	0.50
1:C:397:VAL:HB	1:C:438:PHE:HB3	1.94	0.50
2:J:65:THR:HB	2:J:78:GLN:HB3	1.92	0.50
1:K:328:TYR:CD1	1:K:364:LEU:HD13	2.46	0.50
2:B:11:LEU:HD23	2:B:12:VAL:H	1.76	0.50
2:B:23:THR:HA	2:B:74:THR:HG22	1.93	0.50
1:I:335:VAL:HG13	1:I:368:SER:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:350:VAL:CG1	1:C:364:LEU:HD11	2.42	0.50
2:B:4:LEU:HD11	2:B:94:ALA:HB3	1.93	0.49
1:E:407:VAL:HG22	1:E:505:PHE:HA	1.94	0.49
1:E:362:PHE:HE1	1:E:367:LEU:HD11	1.76	0.49
1:G:368:SER:OG	1:K:496:ARG:NH1	2.44	0.49
2:L:93:ASN:OD1	2:L:104:ASN:ND2	2.42	0.49
2:J:31:MET:HE2	2:J:92:CYS:HB2	1.92	0.49
2:B:64:PHE:HB3	2:B:77:LEU:HD11	1.94	0.49
1:E:326:ILE:HD11	1:E:389:LEU:HD12	1.92	0.49
2:L:94:ALA:O	2:L:104:ASN:HA	2.12	0.49
1:K:399:VAL:HG23	1:K:437:VAL:HG21	1.95	0.49
2:B:64:PHE:CD1	2:B:64:PHE:N	2.81	0.49
1:C:328:TYR:O	1:C:334:GLN:HG3	2.13	0.49
1:K:387:VAL:HG11	1:K:407:VAL:HG21	1.94	0.49
1:A:381:LEU:HD11	1:E:492:VAL:HG12	1.95	0.49
2:L:4:LEU:HD11	2:L:94:ALA:HB3	1.95	0.48
2:J:44:TRP:NE1	2:J:47:SER:OG	2.36	0.48
2:D:31:MET:HB3	2:D:48:ILE:HG22	1.93	0.48
1:E:350:VAL:HG12	1:E:364:LEU:HD11	1.95	0.48
1:K:335:VAL:HG22	1:K:369:ASN:HB2	1.96	0.48
1:K:328:TYR:CE1	1:K:364:LEU:HD13	2.48	0.48
2:D:32:GLY:O	2:D:92:CYS:HA	2.14	0.48
1:E:403:SER:OG	1:E:405:HIS:O	2.31	0.48
1:G:395:GLY:HA3	1:G:440:LEU:HD22	1.95	0.48
1:E:326:ILE:CD1	1:E:389:LEU:HD12	2.44	0.48
1:K:348:VAL:HG12	1:K:389:LEU:O	2.14	0.48
1:E:388:GLN:HB2	1:E:400:ARG:HB3	1.95	0.48
1:C:513:TYR:CD2	3:C:602:ACT:H3	2.47	0.48
1:E:495:LEU:HB3	1:E:536:LEU:HD11	1.94	0.48
2:B:31:MET:O	2:B:47:SER:HB2	2.14	0.47
2:B:99:THR:N	2:B:100:PRO:HD2	2.29	0.47
2:D:23:THR:HG23	2:D:74:THR:CG2	2.44	0.47
1:G:351:ASP:HA	1:G:386:GLY:HA3	1.96	0.47
2:B:60:VAL:O	2:B:62:GLY:N	2.45	0.47
1:E:328:TYR:CD2	1:E:335:VAL:HB	2.49	0.47
2:B:79:MET:HE1	2:B:112:VAL:HG21	1.96	0.47
1:C:408:PHE:CE1	1:C:428:LYS:HG2	2.48	0.47
1:C:408:PHE:HE1	1:C:428:LYS:HG2	1.77	0.47
1:E:354:VAL:HG12	1:E:366:GLN:N	2.30	0.47
1:E:414:LEU:HD11	1:E:437:VAL:HG12	1.95	0.47
2:F:6:GLU:N	2:F:6:GLU:OE1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:33:TRP:CD1	2:F:66:ILE:HD12	2.49	0.47
2:F:59:PHE:CE1	2:F:60:VAL:HG23	2.50	0.47
2:F:28:ILE:HA	2:F:96:ILE:HG22	1.96	0.47
1:G:424:ASP:O	1:G:424:ASP:OD1	2.33	0.47
2:H:60:VAL:O	2:H:60:VAL:HG22	2.14	0.47
2:L:7:SER:O	2:L:20:LEU:HA	2.15	0.47
2:L:10:GLY:N	2:L:111:GLN:O	2.46	0.47
2:D:26:GLY:O	2:D:73:ASN:HB3	2.15	0.47
1:I:368:SER:O	4:I:601:PEG:H42	2.15	0.47
2:F:37:ALA:HB1	2:F:38:PRO:HD2	1.96	0.47
1:I:447:MET:HE1	1:I:536:LEU:HB2	1.97	0.46
2:L:23:THR:HG23	2:L:74:THR:HG22	1.97	0.46
1:C:420:ARG:HD2	1:C:425:ALA:HB2	1.98	0.46
2:B:67:SER:O	2:B:75:VAL:HG13	2.14	0.46
1:C:385:LYS:HE2	1:C:402:LEU:O	2.16	0.46
2:D:65:THR:HB	2:D:78:GLN:HB3	1.97	0.46
1:E:446:GLN:CD	1:E:498:LEU:HD11	2.40	0.46
2:D:31:MET:O	2:D:47:SER:HB2	2.15	0.46
2:D:31:MET:HB3	2:D:48:ILE:CG2	2.46	0.45
1:C:533:LEU:HD22	1:E:354:VAL:HB	1.97	0.45
2:H:31:MET:O	2:H:47:SER:HB2	2.16	0.45
1:I:445:ARG:CZ	2:J:101:GLN:HA	2.45	0.45
1:C:328:TYR:CE1	1:C:364:LEU:HD13	2.51	0.45
1:C:350:VAL:HG12	1:C:364:LEU:HD11	1.99	0.45
2:D:17:SER:HB2	2:D:79:MET:O	2.16	0.45
1:G:444:HIS:ND1	5:G:602:EDO:H12	2.31	0.45
2:J:6:GLU:N	2:J:6:GLU:OE1	2.49	0.45
2:D:34:TYR:CZ	2:D:44:TRP:HD1	2.34	0.45
1:E:341:VAL:CG2	1:E:348:VAL:HG21	2.45	0.45
1:G:418:ALA:HA	2:H:49:THR:HG22	1.99	0.45
1:A:350:VAL:CG1	1:A:364:LEU:HD11	2.46	0.45
1:G:536:LEU:HD23	1:I:354:VAL:HG21	1.99	0.45
2:L:34:TYR:O	2:L:91:TYR:N	2.49	0.45
1:A:397:VAL:HB	1:A:438:PHE:HB3	1.99	0.45
2:H:12:VAL:HG12	2:H:16:GLY:HA3	1.99	0.45
2:H:35:ARG:NH1	2:H:86:ASP:OD1	2.46	0.45
2:B:37:ALA:HB1	2:B:38:PRO:HD2	1.99	0.45
1:G:388:GLN:HB2	1:G:400:ARG:HB3	1.99	0.45
1:C:404:ASP:OD1	1:C:404:ASP:N	2.48	0.45
1:K:326:ILE:HD11	1:K:389:LEU:HD12	1.99	0.45
2:D:37:ALA:HB1	2:D:38:PRO:HD2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:336:GLY:HA3	1:I:367:LEU:HD13	1.98	0.45
1:I:362:PHE:HE1	1:I:367:LEU:HD11	1.82	0.45
1:I:388:GLN:O	1:I:399:VAL:HA	2.17	0.44
2:L:90:TYR:O	2:L:109:GLY:HA2	2.17	0.44
2:F:31:MET:HE2	2:F:92:CYS:HB2	2.00	0.44
1:C:388:GLN:HB2	1:C:400:ARG:HB3	1.99	0.44
2:L:96:ILE:HD11	2:L:105:TYR:CE2	2.52	0.44
1:C:420:ARG:CD	1:C:425:ALA:HB2	2.48	0.44
2:D:28:ILE:HA	2:D:96:ILE:HG22	1.99	0.44
2:F:50:SER:C	2:F:51:THR:HG23	2.43	0.44
1:G:389:LEU:HD13	1:G:527:ILE:HD13	1.99	0.44
1:I:399:VAL:HG23	1:I:437:VAL:HG21	1.99	0.44
1:E:388:GLN:HG3	1:E:402:LEU:HD12	1.99	0.44
2:H:64:PHE:N	2:H:64:PHE:CD1	2.84	0.44
1:C:495:LEU:HB3	1:C:536:LEU:HD11	1.99	0.44
2:H:95:TYR:CE1	2:H:104:ASN:HB2	2.52	0.44
1:I:404:ASP:N	1:I:404:ASP:OD1	2.44	0.44
1:C:429:ILE:HD12	1:C:435:ILE:HG21	1.98	0.44
2:B:2:VAL:HG12	2:B:96:ILE:HD11	1.99	0.43
1:C:453:THR:HG22	1:C:453:THR:O	2.17	0.43
1:C:492:VAL:CA	1:C:495:LEU:HD23	2.41	0.43
2:D:45:VAL:HG12	2:D:45:VAL:O	2.17	0.43
2:B:60:VAL:O	2:B:60:VAL:CG2	2.66	0.43
2:B:18:LEU:HD23	2:B:18:LEU:HA	1.90	0.43
2:B:28:ILE:HA	2:B:96:ILE:HG22	1.99	0.43
2:D:60:VAL:HG21	2:D:64:PHE:CB	2.47	0.43
2:F:23:THR:HG23	2:F:74:THR:HG22	1.99	0.43
2:F:86:ASP:HB2	2:F:114:VAL:HG21	1.99	0.43
1:K:407:VAL:CG1	1:K:503:MET:HG3	2.49	0.43
2:L:37:ALA:HB2	2:L:88:ALA:CB	2.47	0.43
2:H:64:PHE:HA	2:H:78:GLN:O	2.19	0.43
2:B:4:LEU:HD23	2:B:24:ALA:HA	1.99	0.43
2:F:60:VAL:HG11	2:F:64:PHE:HB2	2.01	0.43
2:J:31:MET:O	2:J:47:SER:HB3	2.18	0.43
1:G:381:LEU:HD11	1:K:492:VAL:HG12	2.01	0.43
1:G:493:ASP:HA	1:G:496:ARG:HG2	2.00	0.43
2:L:103:LYS:HG3	2:L:105:TYR:CE2	2.53	0.43
1:A:439:ASP:HB3	1:A:442:GLN:HB3	2.00	0.43
1:G:362:PHE:HE1	1:G:367:LEU:HD11	1.84	0.43
1:C:419:GLY:O	2:D:31:MET:O	2.36	0.43
2:D:33:TRP:CG	2:D:77:LEU:HD22	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:44:TRP:HE1	2:H:47:SER:HB3	1.84	0.43
2:J:2:VAL:HG13	2:J:96:ILE:HD11	1.99	0.43
1:A:420:ARG:HD3	1:A:425:ALA:HB2	2.01	0.43
2:B:17:SER:CB	2:B:80:ASN:HA	2.48	0.43
1:C:502:ARG:NH2	1:C:526:GLU:OE2	2.49	0.43
2:F:7:SER:HB3	2:F:21:SER:HB3	2.00	0.43
2:H:60:VAL:CG2	2:H:64:PHE:H	2.32	0.43
2:J:3:GLN:O	2:J:4:LEU:HD23	2.18	0.43
2:F:12:VAL:HG11	2:F:82:LEU:HD12	2.01	0.42
1:G:350:VAL:CG1	1:G:364:LEU:HD11	2.48	0.42
2:L:20:LEU:HG	2:L:79:MET:HE2	2.00	0.42
2:L:37:ALA:HB1	2:L:38:PRO:HD2	2.00	0.42
1:A:412:TYR:CD2	1:A:498:LEU:HD11	2.55	0.42
1:E:492:VAL:N	1:E:495:LEU:HD23	2.34	0.42
2:F:99:THR:N	2:F:100:PRO:HD2	2.35	0.42
2:B:37:ALA:HB1	2:B:38:PRO:CD	2.49	0.42
1:G:439:ASP:OD1	1:G:441:ARG:N	2.43	0.42
2:H:45:VAL:HG13	2:H:59:PHE:CZ	2.55	0.42
1:K:408:PHE:HB3	1:K:426:VAL:HG12	2.01	0.42
2:D:64:PHE:N	2:D:64:PHE:CD1	2.85	0.42
1:I:322:TYR:HA	1:I:342:PRO:HA	2.01	0.42
1:I:492:VAL:HG12	1:K:381:LEU:HD11	2.00	0.42
1:A:415:ASP:OD2	1:A:423:GLY:N	2.50	0.42
1:E:331:MET:HA	1:E:519:LYS:O	2.19	0.42
1:I:397:VAL:CG1	1:I:438:PHE:HB3	2.48	0.42
2:D:60:VAL:HG21	2:D:64:PHE:CG	2.55	0.42
2:H:95:TYR:HA	2:H:103:LYS:O	2.19	0.42
2:D:7:SER:O	2:D:20:LEU:HA	2.19	0.42
1:G:325:SER:OG	1:G:528:HIS:HB2	2.20	0.42
1:A:388:GLN:HB2	1:A:400:ARG:HB3	2.01	0.41
1:A:399:VAL:O	1:A:434:TYR:HA	2.20	0.41
1:E:409:VAL:HG22	1:E:503:MET:HB2	2.01	0.41
1:A:397:VAL:HG21	1:A:529:LEU:HD22	2.02	0.41
2:B:99:THR:N	2:B:100:PRO:CD	2.84	0.41
1:C:328:TYR:O	1:C:334:GLN:CG	2.67	0.41
1:I:328:TYR:O	1:I:334:GLN:HG3	2.19	0.41
2:D:23:THR:HA	2:D:74:THR:HG22	2.02	0.41
1:E:341:VAL:HG22	1:E:348:VAL:HG21	2.00	0.41
1:G:512:ASP:OD2	2:H:58:ASP:HB2	2.19	0.41
2:H:99:THR:N	2:H:100:PRO:HD2	2.34	0.41
2:D:29:TYR:HB3	2:D:95:TYR:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:45:VAL:HG22	2:H:59:PHE:HZ	1.85	0.41
1:I:416:ARG:NH2	1:I:442:GLN:HG3	2.35	0.41
1:K:328:TYR:O	1:K:334:GLN:HG3	2.19	0.41
1:E:356:PRO:O	1:E:357:SER:C	2.63	0.41
1:G:353:TYR:CD1	1:G:353:TYR:N	2.89	0.41
1:K:397:VAL:HB	1:K:438:PHE:HB3	2.02	0.41
2:L:31:MET:SD	2:L:32:GLY:N	2.94	0.41
1:C:388:GLN:HG3	1:C:402:LEU:HD12	2.02	0.41
1:I:326:ILE:N	1:I:339:PHE:O	2.54	0.41
1:I:387:VAL:CG1	1:I:407:VAL:HG21	2.41	0.41
1:G:445:ARG:O	1:G:449:GLN:HG3	2.21	0.41
2:H:31:MET:HE3	2:H:48:ILE:HG22	2.02	0.41
2:L:101:GLN:HG2	2:L:101:GLN:O	2.20	0.41
2:B:87:SER:O	2:B:88:ALA:HB2	2.19	0.41
2:B:98:THR:CB	2:B:100:PRO:HD2	2.48	0.41
2:F:87:SER:O	2:F:88:ALA:HB2	2.21	0.41
1:I:336:GLY:H	4:I:601:PEG:H31	1.85	0.41
2:J:2:VAL:C	2:J:3:GLN:HG3	2.45	0.41
1:K:407:VAL:HG22	1:K:505:PHE:HA	2.02	0.41
1:E:351:ASP:OD1	1:E:353:TYR:HB2	2.21	0.41
1:I:330:GLU:OE2	1:I:380:ARG:HD2	2.21	0.41
1:I:355:ASP:OD1	1:I:357:SER:HB2	2.20	0.41
1:A:362:PHE:C	1:A:362:PHE:CD1	2.97	0.40
1:A:496:ARG:HD2	1:C:366:GLN:HA	2.03	0.40
1:C:372:ARG:HD3	1:C:377:GLU:HG2	2.03	0.40
1:G:326:ILE:HD11	1:G:389:LEU:HD12	2.01	0.40
1:G:354:VAL:HG21	1:K:536:LEU:HD23	2.02	0.40
2:D:99:THR:HB	2:D:100:PRO:HD3	2.02	0.40
1:G:350:VAL:HG11	1:G:505:PHE:HZ	1.86	0.40
1:G:492:VAL:HA	1:G:495:LEU:HD23	2.02	0.40
1:E:416:ARG:HA	2:F:95:TYR:CE2	2.57	0.40
2:H:56:TYR:OH	2:H:65:THR:HA	2.21	0.40
1:K:388:GLN:HB2	1:K:400:ARG:HB3	2.04	0.40
1:A:414:LEU:HD11	1:A:437:VAL:HG12	2.03	0.40
2:D:79:MET:HB3	2:D:82:LEU:HD21	2.04	0.40
2:L:19:ARG:HA	2:L:77:LEU:O	2.22	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:78:GLN:HE22	1:K:432:SER:O[1_556]	1.49	0.11
2:H:13:GLN:OE1	4:H:201:PEG:O1[1_455]	2.17	0.03
2:B:78:GLN:HE22	1:I:432:SER:O[1_566]	1.59	0.01

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	185/240 (77%)	172 (93%)	13 (7%)	0	100	100
1	C	183/240 (76%)	170 (93%)	12 (7%)	1 (0%)	24	57
1	E	177/240 (74%)	165 (93%)	10 (6%)	2 (1%)	11	39
1	G	186/240 (78%)	173 (93%)	12 (6%)	1 (0%)	24	57
1	I	184/240 (77%)	171 (93%)	12 (6%)	1 (0%)	24	57
1	K	183/240 (76%)	168 (92%)	14 (8%)	1 (0%)	24	57
2	B	111/126 (88%)	103 (93%)	8 (7%)	0	100	100
2	D	107/126 (85%)	96 (90%)	11 (10%)	0	100	100
2	F	110/126 (87%)	104 (94%)	6 (6%)	0	100	100
2	H	111/126 (88%)	102 (92%)	9 (8%)	0	100	100
2	J	103/126 (82%)	96 (93%)	7 (7%)	0	100	100
2	L	90/126 (71%)	87 (97%)	3 (3%)	0	100	100
All	All	1730/2196 (79%)	1607 (93%)	117 (7%)	6 (0%)	36	67

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	395	GLY
1	E	511	PRO
1	G	395	GLY
1	I	422	PRO
1	C	395	GLY

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Mol	Chain	Res	Type
1	K	395	GLY

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	162/191 (85%)	162 (100%)	0	100 100
1	C	161/191 (84%)	161 (100%)	0	100 100
1	E	157/191 (82%)	157 (100%)	0	100 100
1	G	163/191 (85%)	163 (100%)	0	100 100
1	I	161/191 (84%)	160 (99%)	1 (1%)	78 85
1	K	159/191 (83%)	159 (100%)	0	100 100
2	B	91/106 (86%)	91 (100%)	0	100 100
2	D	89/106 (84%)	89 (100%)	0	100 100
2	F	90/106 (85%)	90 (100%)	0	100 100
2	H	90/106 (85%)	90 (100%)	0	100 100
2	J	86/106 (81%)	86 (100%)	0	100 100
2	L	70/106 (66%)	70 (100%)	0	100 100
All	All	1479/1782 (83%)	1478 (100%)	1 (0%)	88 91

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	397	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	444	HIS
1	G	371	HIS
1	G	534	GLN

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Mol	Chain	Res	Type
2	H	36	GLN
1	I	448	GLN
1	K	388	GLN
1	K	427	HIS
1	K	444	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

21 ligands 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	$\#\|Z\| > 2$
4	PEG	I	601	-	6,6,6	0.27	0	5,5,5	0.46	0
5	EDO	E	602	-	3,3,3	0.28	0	2,2,2	0.22	0
3	ACT	E	601	-	3,3,3	1.30	0	3,3,3	1.28	0
5	EDO	A	604	-	3,3,3	0.28	0	2,2,2	0.24	0
4	PEG	G	601	-	6,6,6	0.23	0	5,5,5	0.28	0
3	ACT	J	201	-	3,3,3	1.24	0	3,3,3	1.19	0
4	PEG	A	602	-	6,6,6	0.22	0	5,5,5	0.49	0
3	ACT	C	603	-	3,3,3	1.22	0	3,3,3	1.30	0
3	ACT	C	601	-	3,3,3	1.23	0	3,3,3	1.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	ACT	C	602	-	3,3,3	1.22	0	3,3,3	1.28	0
3	ACT	D	201	-	3,3,3	1.24	0	3,3,3	1.27	0
3	ACT	F	202	-	3,3,3	1.22	0	3,3,3	1.18	0
4	PEG	F	201	-	6,6,6	0.25	0	5,5,5	0.32	0
3	ACT	F	203	-	3,3,3	1.24	0	3,3,3	1.10	0
3	ACT	A	601	-	3,3,3	1.24	0	3,3,3	1.19	0
5	EDO	K	601	-	3,3,3	0.28	0	2,2,2	0.17	0
5	EDO	C	604	-	3,3,3	0.28	0	2,2,2	0.24	0
3	ACT	I	602	-	3,3,3	1.23	0	3,3,3	1.22	0
4	PEG	H	201	-	6,6,6	0.24	0	5,5,5	0.24	0
3	ACT	A	603	-	3,3,3	1.23	0	3,3,3	1.25	0
5	EDO	G	602	-	3,3,3	0.28	0	2,2,2	0.21	0

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
4	PEG	A	602	-	-	1/4/4/4	-
4	PEG	I	601	-	-	1/4/4/4	-
5	EDO	E	602	-	-	0/1/1/1	-
4	PEG	H	201	-	-	1/4/4/4	-
5	EDO	K	601	-	-	1/1/1/1	-
5	EDO	C	604	-	-	1/1/1/1	-
5	EDO	A	604	-	-	1/1/1/1	-
4	PEG	G	601	-	-	2/4/4/4	-
5	EDO	G	602	-	-	0/1/1/1	-
4	PEG	F	201	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	601	PEG	O1-C1-C2-O2
4	I	601	PEG	O1-C1-C2-O2
5	A	604	EDO	O1-C1-C2-O2
4	A	602	PEG	O1-C1-C2-O2
4	G	601	PEG	C1-C2-O2-C3

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Mol	Chain	Res	Type	Atoms
4	H	201	PEG	C1-C2-O2-C3
5	C	604	EDO	O1-C1-C2-O2
5	K	601	EDO	O1-C1-C2-O2
4	F	201	PEG	C4-C3-O2-C2

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	601	PEG	2	0
3	C	602	ACT	5	0
4	H	201	PEG	0	1
5	G	602	EDO	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

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, 95^{th} 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	189/240 (78%)	0.23	3 (1%) 70 47	21, 46, 76, 108	0
1	C	187/240 (77%)	0.55	8 (4%) 40 21	25, 48, 76, 103	0
1	E	181/240 (75%)	0.35	5 (2%) 55 31	21, 42, 74, 93	0
1	G	190/240 (79%)	0.55	11 (5%) 29 14	19, 49, 80, 104	0
1	I	188/240 (78%)	0.37	6 (3%) 50 28	24, 47, 83, 110	0
1	K	187/240 (77%)	0.45	5 (2%) 56 32	28, 53, 82, 113	0
2	B	113/126 (89%)	0.62	6 (5%) 32 16	36, 57, 80, 96	0
2	D	111/126 (88%)	0.99	12 (10%) 11 6	52, 70, 91, 103	0
2	F	112/126 (88%)	0.85	8 (7%) 22 11	39, 80, 106, 124	0
2	H	113/126 (89%)	0.72	13 (11%) 9 5	28, 52, 78, 102	0
2	J	107/126 (84%)	1.02	12 (11%) 10 5	51, 77, 102, 123	0
2	L	98/126 (77%)	1.56	29 (29%) 1 1	60, 85, 105, 116	0
All	All	1776/2196 (80%)	0.61	118 (6%) 24 12	19, 55, 95, 124	0

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	33	TRP	7.3
2	L	28	ILE	5.9
2	J	27	SER	5.6
2	L	90	TYR	5.6
2	L	62	GLY	4.8
2	J	86	ASP	4.5
1	A	456	ALA	4.3
2	J	31	MET	4.2
2	L	77	LEU	4.0
1	G	456	ALA	3.9
2	D	33	TRP	3.8

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Mol	Chain	Res	Type	RSRZ
2	L	70	ASN	3.8
2	D	28	ILE	3.8
2	L	50	SER	3.8
2	L	31	MET	3.7
2	L	39	GLU	3.6
2	L	45	VAL	3.6
2	L	41	GLN	3.6
2	L	36	GLN	3.5
2	J	75	VAL	3.5
2	D	96	ILE	3.5
2	L	22	CYS	3.3
1	C	319	ALA	3.3
2	H	28	ILE	3.3
2	H	33	TRP	3.3
2	L	88	ALA	3.3
1	C	354	VAL	3.3
2	H	53	ASN	3.2
2	J	61	ASN	3.2
2	H	75	VAL	3.2
1	G	381	LEU	3.2
2	D	82	LEU	3.1
2	D	61	ASN	3.1
1	E	335	VAL	3.1
2	D	49	THR	3.1
2	F	96	ILE	3.0
1	G	426	VAL	3.0
2	L	66	ILE	3.0
1	I	455	GLN	3.0
2	J	77	LEU	3.0
1	K	335	VAL	2.9
2	D	85	GLU	2.9
1	K	514	PRO	2.8
2	J	66	ILE	2.8
2	D	112	VAL	2.8
2	L	67	SER	2.8
2	F	99	THR	2.8
1	K	512	ASP	2.8
2	H	96	ILE	2.8
2	F	15	GLY	2.8
2	L	76	TYR	2.7
1	E	336	GLY	2.7
2	L	20	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
2	H	92	CYS	2.7
2	J	35	ARG	2.6
2	H	20	LEU	2.6
1	I	394	GLU	2.6
2	H	49	THR	2.6
2	J	33	TRP	2.6
1	C	416	ARG	2.6
1	I	514	PRO	2.6
2	L	64	PHE	2.6
2	L	79	MET	2.6
2	L	94	ALA	2.6
2	L	48	ILE	2.6
2	H	70	ASN	2.6
2	H	93	ASN	2.6
1	E	381	LEU	2.6
2	H	77	LEU	2.6
1	G	520	GLU	2.6
2	F	48	ILE	2.5
2	H	50	SER	2.5
1	E	501	LEU	2.5
2	F	86	ASP	2.5
2	H	32	GLY	2.5
1	G	506	VAL	2.5
2	B	51	THR	2.5
1	C	522	PRO	2.5
2	L	81	SER	2.4
2	F	105	TYR	2.4
1	G	335	VAL	2.4
1	E	529	LEU	2.4
2	L	99	THR	2.4
1	G	447	MET	2.4
1	C	345	CYS	2.4
2	F	66	ILE	2.3
1	A	543	MET	2.3
1	G	345	CYS	2.3
2	D	67	SER	2.3
1	I	381	LEU	2.3
2	J	43	GLU	2.3
2	B	62	GLY	2.3
2	B	13	GLN	2.3
1	G	425	ALA	2.2
1	I	319	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
2	F	60	VAL	2.2
1	C	539	VAL	2.2
2	L	29	TYR	2.2
2	D	7	SER	2.2
2	D	50	SER	2.2
1	C	381	LEU	2.2
2	J	20	LEU	2.2
2	B	31	MET	2.2
2	L	69	ASP	2.2
2	L	63	ARG	2.1
1	I	506	VAL	2.1
1	G	516	GLN	2.1
2	L	42	ARG	2.1
2	D	45	VAL	2.1
2	J	28	ILE	2.1
2	B	28	ILE	2.1
1	C	523	CYS	2.1
1	K	454	ALA	2.1
2	B	95	TYR	2.0
2	L	54	SER	2.0
1	A	375	ALA	2.0
1	G	383	ILE	2.0
1	K	435	ILE	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (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, 95^{th} 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ACT	D	201	4/4	0.54	0.27	38,47,57,66	0
3	ACT	I	602	4/4	0.68	0.21	40,49,49,54	0
3	ACT	F	203	4/4	0.70	0.25	44,50,61,61	0
5	EDO	K	601	4/4	0.71	0.24	60,73,77,77	0
4	PEG	F	201	7/7	0.73	0.16	48,61,89,89	0
4	PEG	G	601	7/7	0.76	0.12	15,32,39,39	0
3	ACT	F	202	4/4	0.76	0.26	45,57,70,70	0
3	ACT	A	601	4/4	0.78	0.21	42,51,59,69	0
3	ACT	J	201	4/4	0.79	0.30	45,60,73,73	0
5	EDO	C	604	4/4	0.81	0.14	37,59,76,92	0
3	ACT	E	601	4/4	0.82	0.19	40,44,48,50	0
4	PEG	I	601	7/7	0.82	0.21	48,65,76,89	0
5	EDO	E	602	4/4	0.84	0.18	20,26,36,44	0
3	ACT	C	601	4/4	0.85	0.21	30,37,38,45	0
5	EDO	G	602	4/4	0.87	0.17	41,62,75,75	0
4	PEG	H	201	7/7	0.87	0.15	37,61,80,80	0
3	ACT	A	603	4/4	0.88	0.12	22,40,58,58	0
5	EDO	A	604	4/4	0.89	0.10	32,41,55,55	0
4	PEG	A	602	7/7	0.91	0.12	25,37,70,70	0
3	ACT	C	603	4/4	0.97	0.07	5,18,54,54	0
3	ACT	C	602	4/4	0.98	0.07	16,49,59,59	0

6.5 Other polymers (i)

There are no such residues in this entry.