



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:54 AM UTC

PDB ID : 6QL4 / pdb_00006ql4
Title : Crystal structure of nucleotide-free Mgm1
Authors : Faelber, K.; Dietrich, L.; Noel, J.K.; Wollweber, F.; Pfitzner, A.-K.; Muehleip, A.; Sanchez, R.; Kudryashev, M.; Chiaruttin, N.; Lilie, H.; Schlegel, J.; Rosenbaum, E.; Hessenberger, M.; Matthaeus, C.; Noe, F.; Roux, A.; vanderLaan, M.; Kuehlbrandt, W.; Daumke, O.
Deposited on : 2019-01-31
Resolution : 3.60 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

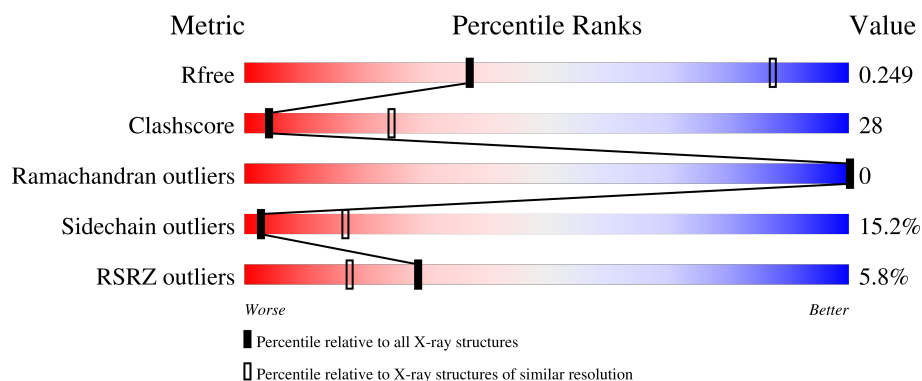
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

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	939	3% 49% 17% • 30%
1	B	939	5% 41% 21% 8% 30%

2 Entry composition [i](#)

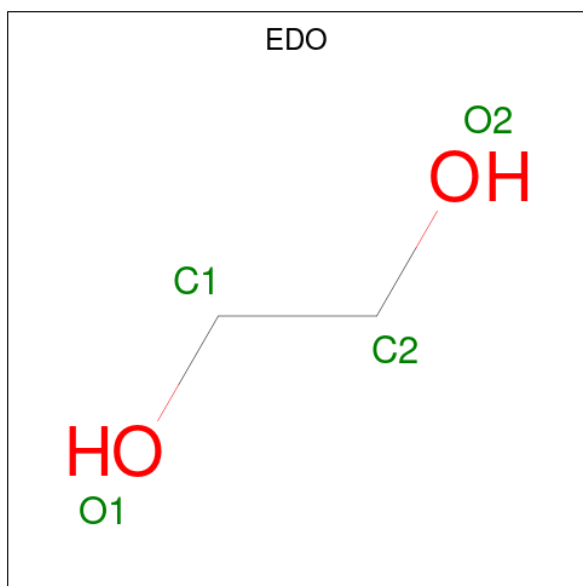
There are 2 unique types of molecules in this entry. The entry contains 10330 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Putative mitochondrial dynamin protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	660	Total	C	N	O	S	Se	0	0	0
			5163	3249	914	983	5	12			
1	B	660	Total	C	N	O	S	Se	0	0	0
			5159	3247	911	984	5	12			

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	147.40Å 147.40Å 344.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.13 – 3.60 49.13 – 3.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.13-3.60) 99.8 (49.13-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 3.57Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.243 , 0.252 0.245 , 0.249	Depositor DCC
R_{free} test set	2242 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	113.6	Xtriage
Anisotropy	0.005	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 66.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10330	wwPDB-VP
Average B, all atoms (Å ²)	146.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: EDO

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	0.18	0/5237	0.41	2/7053 (0.0%)
1	B	0.53	1/5233 (0.0%)	0.81	26/7049 (0.4%)
All	All	0.40	1/10470 (0.0%)	0.64	28/14102 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	253	PRO	C-N	-15.98	1.13	1.33

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	445	GLN	CA-C-N	-10.73	112.39	122.37
1	B	445	GLN	C-N-CA	-10.73	112.39	122.37
1	B	440	ILE	N-CA-C	9.91	119.85	110.53
1	B	500	THR	N-CA-C	9.85	123.85	108.79
1	B	483	ASN	N-CA-C	9.23	121.42	111.36
1	B	227	MSE	N-CA-C	8.74	120.58	111.14
1	B	244	VAL	N-CA-C	8.73	118.80	110.42
1	B	244	VAL	CB-CA-C	-8.69	100.85	111.97
1	B	496	SER	N-CA-C	-8.16	98.99	110.50
1	B	262	SER	N-CA-C	-7.78	102.74	111.14
1	B	435	GLU	N-CA-C	-7.11	103.53	111.28
1	B	251	THR	N-CA-C	7.00	118.83	108.60
1	A	610	ARG	CA-C-N	6.70	128.46	120.09
1	A	610	ARG	C-N-CA	6.70	128.46	120.09
1	B	250	VAL	N-CA-C	6.69	119.26	109.63
1	B	224	ASP	CA-C-N	6.66	129.75	120.29
1	B	224	ASP	C-N-CA	6.66	129.75	120.29
1	B	234	MSE	CB-CG-SE	-6.17	94.19	112.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	228	MSE	N-CA-C	-6.13	104.68	111.36
1	B	438	ALA	CA-C-N	-6.06	112.20	120.44
1	B	438	ALA	C-N-CA	-6.06	112.20	120.44
1	B	484	TYR	N-CA-C	5.97	117.79	111.28
1	B	405	ASN	N-CA-C	5.57	117.35	111.28
1	B	252	LEU	CA-C-N	-5.54	114.89	120.21
1	B	252	LEU	C-N-CA	-5.54	114.89	120.21
1	B	249	THR	N-CA-C	-5.50	105.36	111.36
1	B	493	GLY	CA-C-N	-5.21	114.36	119.93
1	B	493	GLY	C-N-CA	-5.21	114.36	119.93

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	5163	0	5236	107	1
1	B	5159	0	5228	471	1
2	A	4	0	6	0	0
2	B	4	0	6	0	0
All	All	10330	0	10476	576	1

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 28.

All (576) 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:B:426:ILE:CD1	1:B:440:ILE:HG22	1.20	1.67
1:B:441:LEU:CD2	1:B:498:VAL:HB	1.31	1.61
1:B:426:ILE:HD13	1:B:440:ILE:CG2	1.35	1.56
1:B:441:LEU:HD23	1:B:498:VAL:CB	1.14	1.53
1:B:478:ASN:ND2	1:B:482:LYS:HZ3	1.21	1.39
1:B:260:SER:O	1:B:264:GLY:N	1.58	1.35

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:445:GLN:O	1:B:446:TYR:CD1	1.82	1.33
1:B:269:LEU:HD21	1:B:457:SER:CB	1.60	1.32
1:B:426:ILE:CD1	1:B:440:ILE:CG2	1.97	1.29
1:B:272:ILE:HG23	1:B:278:LEU:CD1	1.66	1.24
1:B:287:ARG:HD2	1:B:332:VAL:CG1	1.65	1.24
1:B:441:LEU:HD23	1:B:498:VAL:CG1	1.65	1.23
1:B:269:LEU:HD11	1:B:457:SER:O	1.04	1.21
1:B:478:ASN:CG	1:B:482:LYS:NZ	1.99	1.21
1:B:297:ASP:CG	1:B:300:ALA:HB3	1.65	1.20
1:B:285:ILE:HG12	1:B:332:VAL:HG22	1.21	1.19
1:B:287:ARG:CD	1:B:332:VAL:CG1	2.20	1.19
1:B:426:ILE:HD11	1:B:440:ILE:HG22	1.23	1.17
1:B:478:ASN:ND2	1:B:482:LYS:NZ	1.92	1.16
1:B:478:ASN:CG	1:B:482:LYS:HZ1	1.53	1.16
1:B:269:LEU:CD1	1:B:457:SER:O	1.93	1.15
1:B:287:ARG:HH11	1:B:332:VAL:HG11	1.11	1.13
1:B:287:ARG:CD	1:B:332:VAL:HG13	1.79	1.11
1:B:269:LEU:CD2	1:B:457:SER:OG	2.00	1.09
1:B:278:LEU:CD2	1:B:280:LYS:HD3	1.81	1.09
1:B:297:ASP:OD2	1:B:300:ALA:HB3	1.51	1.08
1:B:284:MSE:HG2	1:B:286:THR:HG23	1.29	1.08
1:B:278:LEU:HD21	1:B:280:LYS:CD	1.83	1.07
1:B:272:ILE:HG23	1:B:278:LEU:HD12	1.07	1.07
1:B:441:LEU:HG	1:B:498:VAL:HG12	1.34	1.06
1:B:441:LEU:CD2	1:B:498:VAL:CB	2.05	1.05
1:B:426:ILE:HD13	1:B:440:ILE:HG21	1.14	1.05
1:B:246:GLN:N	1:B:246:GLN:OE1	1.91	1.04
1:B:443:ASP:OD1	1:B:445:GLN:N	1.88	1.04
1:B:458:LYS:O	1:B:458:LYS:NZ	1.90	1.04
1:B:285:ILE:HG12	1:B:332:VAL:CG2	1.87	1.04
1:B:269:LEU:CD2	1:B:457:SER:CB	2.35	1.03
1:B:269:LEU:HD21	1:B:457:SER:OG	1.57	1.03
1:B:279:PRO:HG2	1:B:325:LEU:HD21	1.36	1.03
1:B:287:ARG:HD2	1:B:332:VAL:HG13	1.36	1.03
1:B:307:PHE:CE1	1:B:345:LEU:HD21	1.93	1.02
1:B:278:LEU:HD21	1:B:280:LYS:HD3	1.03	1.02
1:B:287:ARG:HD2	1:B:332:VAL:HG11	1.39	1.01
1:B:269:LEU:HA	1:B:272:ILE:HD12	1.41	0.99
1:B:441:LEU:CG	1:B:498:VAL:HG12	1.93	0.99
1:B:273:VAL:HG21	1:B:457:SER:HB3	1.44	0.99
1:B:273:VAL:HG11	1:B:457:SER:HB2	1.43	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:441:LEU:HD21	1:B:499:SER:H	1.27	0.97
1:B:430:ASP:C	1:B:430:ASP:OD1	2.06	0.96
1:B:251:THR:HG22	1:B:252:LEU:H	1.30	0.96
1:B:376:LYS:HZ2	1:B:379:ILE:HD12	1.28	0.96
1:B:363:TYR:HE1	1:B:383:CYS:SG	1.88	0.95
1:B:488:HIS:HB3	1:B:491:GLU:HG2	1.47	0.95
1:B:441:LEU:HD21	1:B:499:SER:N	1.81	0.95
1:B:269:LEU:HD21	1:B:457:SER:HB2	1.46	0.94
1:B:490:THR:OG1	1:B:491:GLU:OE2	1.85	0.94
1:B:376:LYS:NZ	1:B:376:LYS:HA	1.83	0.94
1:B:272:ILE:HG22	1:B:277:PHE:HA	1.48	0.93
1:B:429:MSE:HE2	1:B:437:GLY:HA2	1.48	0.93
1:B:272:ILE:CG2	1:B:278:LEU:HD12	1.98	0.92
1:B:269:LEU:CD2	1:B:457:SER:HB2	1.99	0.92
1:B:226:ASN:C	1:B:229:PHE:CD1	2.33	0.92
1:B:441:LEU:CD2	1:B:498:VAL:CG1	2.40	0.92
1:B:297:ASP:CG	1:B:300:ALA:CB	2.41	0.92
1:B:445:GLN:O	1:B:446:TYR:HD1	1.39	0.92
1:B:426:ILE:HD12	1:B:440:ILE:HG22	1.47	0.91
1:B:287:ARG:HD3	1:B:332:VAL:CG1	1.96	0.91
1:B:434:PRO:CB	1:B:491:GLU:HG3	1.99	0.91
1:B:485:PHE:CD2	1:B:492:PHE:CD1	2.59	0.91
1:B:226:ASN:C	1:B:229:PHE:HD1	1.73	0.91
1:B:455:VAL:HG12	1:B:501:GLY:H	1.34	0.91
1:B:284:MSE:HG2	1:B:286:THR:CG2	2.00	0.90
1:B:297:ASP:OD1	1:B:300:ALA:CB	2.19	0.90
1:B:286:THR:HB	1:B:361:PRO:HB3	1.51	0.90
1:B:485:PHE:CE2	1:B:500:THR:OG1	2.27	0.88
1:B:376:LYS:NZ	1:B:379:ILE:HD12	1.87	0.87
1:B:278:LEU:HD22	1:B:279:PRO:O	1.75	0.87
1:B:486:GLY:O	1:B:489:PRO:HD3	1.74	0.87
1:B:269:LEU:O	1:B:273:VAL:HG13	1.75	0.86
1:B:279:PRO:HB3	1:B:322:GLN:CB	2.06	0.85
1:B:433:GLU:O	1:B:436:LYS:HB2	1.77	0.85
1:B:478:ASN:HD21	1:B:482:LYS:HZ3	1.20	0.85
1:B:485:PHE:HD2	1:B:492:PHE:O	1.58	0.85
1:B:287:ARG:HH11	1:B:332:VAL:CG1	1.88	0.85
1:B:285:ILE:CG1	1:B:332:VAL:HG22	2.05	0.84
1:B:234:MSE:O	1:B:237:ILE:HG22	1.76	0.84
1:B:383:CYS:O	1:B:387:ILE:HG13	1.78	0.84
1:B:285:ILE:HD12	1:B:285:ILE:O	1.77	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:ILE:O	1:B:286:THR:OG1	1.96	0.83
1:B:241:LEU:O	1:B:244:VAL:HG23	1.79	0.83
1:B:453:VAL:HG11	1:B:505:LEU:HB2	1.61	0.83
1:B:430:ASP:OD1	1:B:430:ASP:O	1.96	0.82
1:B:485:PHE:CZ	1:B:500:THR:OG1	2.31	0.82
1:B:297:ASP:OD2	1:B:300:ALA:CB	2.28	0.82
1:B:251:THR:HG22	1:B:252:LEU:N	1.88	0.81
1:B:434:PRO:HG2	1:B:488:HIS:CG	2.14	0.81
1:B:488:HIS:HB3	1:B:491:GLU:CG	2.10	0.81
1:B:434:PRO:HB3	1:B:491:GLU:HG3	1.62	0.81
1:B:287:ARG:NH1	1:B:332:VAL:HG11	1.94	0.80
1:A:285:ILE:HD12	1:A:287:ARG:H	1.47	0.80
1:B:225:ASP:N	1:B:225:ASP:OD1	2.10	0.79
1:B:272:ILE:CG2	1:B:278:LEU:CD1	2.55	0.79
1:B:285:ILE:CG2	1:B:329:ASN:O	2.30	0.79
1:B:441:LEU:CG	1:B:498:VAL:CG1	2.60	0.79
1:B:267:SER:HB3	1:B:396:ILE:HG13	1.66	0.77
1:B:235:ILE:HD12	1:B:235:ILE:O	1.84	0.77
1:B:244:VAL:HB	1:B:248:SER:OG	1.84	0.77
1:B:257:VAL:CG2	1:B:359:ASP:HA	2.14	0.77
1:B:279:PRO:CB	1:B:322:GLN:HA	2.14	0.77
1:A:260:SER:O	1:A:264:GLY:N	2.19	0.76
1:B:237:ILE:HD13	1:B:237:ILE:O	1.86	0.76
1:A:224:ASP:HB3	1:A:227:MSE:HB2	1.68	0.76
1:B:284:MSE:H	1:B:284:MSE:SE	2.19	0.76
1:B:377:ARG:HH21	1:B:377:ARG:HG2	1.51	0.76
1:B:441:LEU:HB3	1:B:498:VAL:HG11	1.66	0.76
1:B:388:ARG:O	1:B:421:ARG:NH2	2.18	0.76
1:B:572:PHE:O	1:B:576:GLN:NE2	2.19	0.76
1:B:308:PRO:HG3	1:B:344:ARG:HB2	1.68	0.75
1:B:443:ASP:OD1	1:B:444:ARG:N	2.19	0.75
1:B:273:VAL:HG11	1:B:457:SER:CB	2.14	0.75
1:B:363:TYR:CE1	1:B:383:CYS:SG	2.71	0.75
1:B:376:LYS:HA	1:B:376:LYS:HZ1	1.52	0.75
1:B:270:GLU:O	1:B:273:VAL:HG22	1.87	0.75
1:B:480:ASN:HA	1:B:483:ASN:OD1	1.86	0.74
1:B:229:PHE:HA	1:B:232:LYS:HG2	1.68	0.74
1:B:310:LEU:N	1:B:310:LEU:HD23	2.02	0.74
1:B:493:GLY:O	1:B:496:SER:HB3	1.86	0.74
1:B:285:ILE:HD11	1:B:287:ARG:HB2	1.68	0.74
1:B:272:ILE:HG21	1:B:277:PHE:CD1	2.24	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:LEU:N	1:B:240:LEU:HD23	2.03	0.73
1:B:226:ASN:O	1:B:229:PHE:HD1	1.71	0.73
1:B:286:THR:O	1:B:361:PRO:HG3	1.89	0.73
1:B:434:PRO:HG2	1:B:488:HIS:ND1	2.04	0.73
1:B:434:PRO:HB3	1:B:491:GLU:CG	2.18	0.73
1:B:472:ASN:HD21	1:B:475:ALA:HB3	1.52	0.73
1:A:843:VAL:O	1:A:847:ASN:HB2	1.89	0.73
1:B:224:ASP:CG	1:B:227:MSE:HB2	2.14	0.72
1:B:455:VAL:HG12	1:B:501:GLY:N	2.02	0.72
1:B:485:PHE:CD2	1:B:492:PHE:HD1	2.07	0.72
1:B:640:THR:HG21	1:B:706:LYS:HA	1.70	0.72
1:B:269:LEU:HD21	1:B:457:SER:CA	2.19	0.72
1:B:287:ARG:HD3	1:B:332:VAL:HG13	1.61	0.72
1:B:339:THR:HG23	1:B:340:ASP:N	2.05	0.71
1:B:375:LEU:N	1:B:375:LEU:HD23	2.03	0.71
1:B:307:PHE:CE1	1:B:345:LEU:CD2	2.73	0.71
1:B:269:LEU:HD23	1:B:270:GLU:N	2.05	0.71
1:B:278:LEU:CD2	1:B:280:LYS:CD	2.54	0.71
1:B:265:LYS:O	1:B:268:VAL:HG23	1.91	0.71
1:B:454:GLY:O	1:B:500:THR:HB	1.91	0.71
1:B:269:LEU:HD23	1:B:269:LEU:C	2.16	0.70
1:A:642:LEU:HD22	1:A:643:GLY:H	1.55	0.70
1:B:279:PRO:HB3	1:B:322:GLN:HA	1.74	0.70
1:B:275:HIS:CG	1:B:276:GLU:H	2.09	0.70
1:B:286:THR:O	1:B:361:PRO:CG	2.40	0.70
1:B:260:SER:N	1:B:263:SER:HB3	2.07	0.70
1:B:279:PRO:HB3	1:B:322:GLN:HB2	1.71	0.70
1:B:269:LEU:HD11	1:B:457:SER:C	2.09	0.69
1:B:279:PRO:O	1:B:280:LYS:HD2	1.92	0.69
1:B:878:ASP:HB3	1:B:881:VAL:HG22	1.74	0.69
1:B:285:ILE:HG13	1:B:287:ARG:CB	2.22	0.69
1:B:339:THR:HG23	1:B:340:ASP:H	1.57	0.69
1:B:690:ARG:NH1	1:B:844:GLU:OE2	2.26	0.69
1:B:285:ILE:HG13	1:B:287:ARG:H	1.56	0.69
1:B:694:THR:HG21	1:B:845:MSE:HB2	1.73	0.69
1:B:499:SER:O	1:B:500:THR:HG23	1.93	0.69
1:B:279:PRO:HB3	1:B:322:GLN:CA	2.22	0.69
1:B:286:THR:O	1:B:361:PRO:HB3	1.93	0.69
1:B:445:GLN:C	1:B:446:TYR:CD1	2.69	0.68
1:B:499:SER:O	1:B:500:THR:CG2	2.41	0.68
1:B:278:LEU:HB2	1:B:279:PRO:HD2	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:279:PRO:HG2	1:B:325:LEU:CD2	2.21	0.68
1:B:473:LEU:O	1:B:476:SER:OG	2.05	0.68
1:A:687:LEU:HD22	1:A:845:MSE:HE2	1.76	0.68
1:B:231:THR:O	1:B:235:ILE:HG22	1.94	0.68
1:B:278:LEU:HD13	1:B:278:LEU:O	1.94	0.68
1:B:272:ILE:HG23	1:B:278:LEU:H	1.58	0.68
1:B:272:ILE:CG2	1:B:278:LEU:H	2.05	0.67
1:B:434:PRO:HB2	1:B:491:GLU:HG3	1.76	0.67
1:B:272:ILE:HG23	1:B:278:LEU:HD13	1.70	0.67
1:B:472:ASN:ND2	1:B:475:ALA:HB3	2.10	0.67
1:A:434:PRO:HG2	1:A:488:HIS:CG	2.30	0.66
1:B:278:LEU:CD2	1:B:280:LYS:CG	2.73	0.66
1:B:229:PHE:O	1:B:233:LYS:HG2	1.95	0.66
1:A:429:MSE:HE2	1:A:437:GLY:HA2	1.78	0.66
1:B:273:VAL:CG1	1:B:457:SER:HB2	2.23	0.66
1:B:279:PRO:O	1:B:280:LYS:CD	2.44	0.66
1:B:434:PRO:HB3	1:B:491:GLU:CB	2.25	0.66
1:A:863:GLU:O	1:A:867:ALA:HB3	1.96	0.66
1:B:230:ILE:O	1:B:234:MSE:HG3	1.96	0.66
1:B:272:ILE:CG2	1:B:277:PHE:HA	2.25	0.66
1:B:278:LEU:HD22	1:B:280:LYS:HG2	1.78	0.66
1:B:272:ILE:HG21	1:B:277:PHE:HD1	1.61	0.65
1:B:273:VAL:HG21	1:B:457:SER:CB	2.23	0.65
1:B:657:GLN:HE22	1:B:684:ALA:HA	1.61	0.65
1:B:238:ARG:NH2	1:B:356:SER:OG	2.30	0.65
1:A:285:ILE:HD13	1:A:332:VAL:HG22	1.78	0.64
1:A:387:ILE:O	1:A:421:ARG:NH2	2.29	0.64
1:B:257:VAL:HG22	1:B:359:ASP:HA	1.79	0.64
1:B:232:LYS:HA	1:B:235:ILE:CG2	2.28	0.64
1:B:396:ILE:HG22	1:B:425:VAL:HB	1.79	0.64
1:B:434:PRO:CG	1:B:488:HIS:CG	2.81	0.64
1:B:441:LEU:HD23	1:B:498:VAL:HB	0.65	0.64
1:B:285:ILE:HG21	1:B:329:ASN:O	1.97	0.64
1:B:242:GLN:HE22	1:B:344:ARG:HD2	1.62	0.64
1:B:285:ILE:HD12	1:B:285:ILE:C	2.21	0.64
1:B:297:ASP:OD1	1:B:300:ALA:HB3	1.89	0.64
1:B:456:ILE:O	1:B:481:GLU:OE2	2.16	0.64
1:B:278:LEU:HD21	1:B:280:LYS:CG	2.27	0.64
1:B:485:PHE:CD2	1:B:492:PHE:O	2.47	0.64
1:B:278:LEU:CD2	1:B:280:LYS:HG2	2.27	0.64
1:A:429:MSE:HE1	1:A:441:LEU:HB2	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:667:SER:OG	1:A:668:SER:N	2.32	0.63
1:A:249:THR:OG1	1:A:531:GLU:OE1	2.13	0.63
1:A:578:GLN:HA	1:A:838:VAL:HG21	1.80	0.63
1:B:363:TYR:CD1	1:B:363:TYR:N	2.66	0.63
1:B:277:PHE:HD1	1:B:278:LEU:H	1.46	0.63
1:B:363:TYR:CD2	1:B:407:THR:HB	2.33	0.63
1:B:237:ILE:HD12	1:B:241:LEU:HD11	1.81	0.63
1:B:285:ILE:CD1	1:B:287:ARG:HB2	2.29	0.63
1:B:252:LEU:HD23	1:B:524:THR:HG21	1.81	0.63
1:B:268:VAL:O	1:B:272:ILE:HG13	1.99	0.63
1:A:322:GLN:O	1:A:326:THR:OG1	2.14	0.62
1:B:269:LEU:HD21	1:B:457:SER:C	2.24	0.62
1:A:843:VAL:HG21	1:B:704:PRO:HA	1.80	0.62
1:B:294:LEU:HB3	1:B:352:ILE:HD13	1.81	0.62
1:B:224:ASP:OD1	1:B:227:MSE:HB2	2.00	0.62
1:B:298:PRO:O	1:B:299:GLU:HB3	1.97	0.62
1:B:458:LYS:HZ3	1:B:458:LYS:C	1.99	0.62
1:B:491:GLU:OE2	1:B:491:GLU:N	2.33	0.62
1:B:617:ASP:N	1:B:617:ASP:OD1	2.33	0.62
1:B:272:ILE:HG12	1:B:278:LEU:HD11	1.82	0.62
1:B:526:GLU:OE1	1:B:530:ARG:NH1	2.32	0.62
1:B:441:LEU:HB3	1:B:498:VAL:CG1	2.30	0.62
1:A:308:PRO:HG3	1:A:344:ARG:HB2	1.82	0.61
1:B:287:ARG:HD3	1:B:332:VAL:HG12	1.81	0.61
1:A:524:THR:O	1:A:528:ILE:HG13	2.01	0.61
1:B:576:GLN:NE2	1:B:576:GLN:H	1.97	0.61
1:B:272:ILE:HG12	1:B:278:LEU:CD1	2.30	0.61
1:B:284:MSE:HE2	1:B:284:MSE:O	2.00	0.61
1:B:230:ILE:HG13	1:B:904:LEU:HD11	1.83	0.61
1:B:377:ARG:HH21	1:B:377:ARG:CG	2.14	0.61
1:B:233:LYS:HE3	1:B:233:LYS:N	2.15	0.60
1:B:376:LYS:HA	1:B:376:LYS:CE	2.30	0.60
1:B:456:ILE:HD12	1:B:457:SER:N	2.15	0.60
1:A:286:THR:HB	1:A:361:PRO:HB3	1.84	0.60
1:B:485:PHE:HA	1:B:492:PHE:HE1	1.66	0.60
1:A:258:ILE:HG22	1:A:360:LEU:HD11	1.83	0.60
1:B:277:PHE:HD1	1:B:278:LEU:N	1.99	0.60
1:B:308:PRO:HG3	1:B:344:ARG:HG3	1.83	0.60
1:B:524:THR:O	1:B:528:ILE:HG13	2.02	0.60
1:B:276:GLU:OE1	1:B:303:ASP:CG	2.44	0.60
1:A:690:ARG:NH1	1:A:844:GLU:OE2	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:279:PRO:CG	1:B:325:LEU:HD21	2.22	0.60
1:B:233:LYS:HE2	1:B:233:LYS:HA	1.84	0.60
1:B:665:ASP:OD1	1:B:676:ARG:NH2	2.34	0.60
1:B:232:LYS:HG3	1:B:233:LYS:HE3	1.83	0.59
1:B:238:ARG:HA	1:B:241:LEU:HD12	1.85	0.59
1:B:363:TYR:N	1:B:363:TYR:HD1	1.99	0.59
1:B:232:LYS:O	1:B:235:ILE:HG23	2.02	0.59
1:B:297:ASP:HB3	1:B:349:SER:C	2.28	0.59
1:A:863:GLU:O	1:A:867:ALA:CB	2.51	0.59
1:B:423:ILE:HG22	1:B:450:LEU:HD13	1.84	0.59
1:A:640:THR:HG22	1:A:706:LYS:HG2	1.85	0.58
1:A:576:GLN:N	1:A:576:GLN:OE1	2.36	0.58
1:A:878:ASP:HB3	1:A:881:VAL:HG12	1.85	0.58
1:B:387:ILE:CG2	1:B:415:VAL:HG21	2.34	0.58
1:B:441:LEU:CD2	1:B:498:VAL:CA	2.81	0.58
1:B:263:SER:HA	1:B:266:SER:OG	2.03	0.58
1:B:285:ILE:HG13	1:B:287:ARG:HB3	1.84	0.58
1:B:263:SER:OG	1:B:397:SER:HA	2.03	0.58
1:B:276:GLU:HG2	1:B:277:PHE:N	2.19	0.58
1:B:454:GLY:O	1:B:500:THR:CG2	2.52	0.58
1:B:286:THR:O	1:B:361:PRO:CB	2.52	0.58
1:B:574:ARG:H	1:B:575:PRO:HD2	1.67	0.58
1:B:242:GLN:HE22	1:B:344:ARG:CD	2.16	0.57
1:B:251:THR:CG2	1:B:252:LEU:H	2.11	0.57
1:B:454:GLY:O	1:B:500:THR:CB	2.52	0.57
1:B:229:PHE:HA	1:B:232:LYS:CG	2.34	0.57
1:B:441:LEU:CD2	1:B:498:VAL:HG12	2.17	0.57
1:B:277:PHE:CD1	1:B:278:LEU:N	2.73	0.57
1:B:269:LEU:HA	1:B:272:ILE:CD1	2.27	0.57
1:A:259:GLY:HA2	1:A:408:ALA:HB2	1.87	0.57
1:B:275:HIS:CD2	1:B:275:HIS:H	2.22	0.56
1:A:665:ASP:OD1	1:A:676:ARG:NH1	2.38	0.56
1:B:255:ILE:HD11	1:B:355:LEU:HG	1.87	0.56
1:B:275:HIS:CG	1:B:276:GLU:N	2.72	0.56
1:B:296:ASN:C	1:B:298:PRO:HD3	2.30	0.56
1:B:382:LEU:HD12	1:B:382:LEU:C	2.30	0.56
1:B:610:ARG:HE	1:B:610:ARG:HA	1.70	0.56
1:B:284:MSE:SE	1:B:284:MSE:N	2.89	0.56
1:B:667:SER:OG	1:B:668:SER:N	2.36	0.56
1:A:661:GLU:OE2	1:A:676:ARG:NH2	2.39	0.56
1:B:272:ILE:CG2	1:B:277:PHE:HD1	2.18	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:LEU:CA	1:B:272:ILE:HD12	2.27	0.55
1:B:339:THR:O	1:B:340:ASP:HB3	2.06	0.55
1:B:441:LEU:HD21	1:B:498:VAL:HB	1.67	0.55
1:B:264:GLY:O	1:B:268:VAL:HG22	2.07	0.55
1:B:307:PHE:CD1	1:B:345:LEU:CD2	2.89	0.55
1:A:653:ALA:HB2	1:A:845:MSE:HE1	1.88	0.55
1:B:258:ILE:HG22	1:B:360:LEU:HD11	1.89	0.55
1:B:269:LEU:HD11	1:B:458:LYS:HB2	1.89	0.55
1:B:363:TYR:HD2	1:B:407:THR:HB	1.71	0.55
1:A:297:ASP:HB3	1:A:349:SER:C	2.32	0.55
1:B:285:ILE:CG1	1:B:287:ARG:HB2	2.37	0.55
1:A:585:LEU:HD12	1:A:834:ALA:HB2	1.89	0.55
1:B:270:GLU:HA	1:B:273:VAL:HG22	1.87	0.55
1:B:276:GLU:OE1	1:B:303:ASP:OD1	2.25	0.55
1:B:485:PHE:HZ	1:B:500:THR:HG1	1.39	0.55
1:B:308:PRO:HG3	1:B:344:ARG:CB	2.37	0.54
1:B:436:LYS:O	1:B:440:ILE:HG13	2.07	0.54
1:A:383:CYS:O	1:A:387:ILE:HG13	2.06	0.54
1:B:257:VAL:HG22	1:B:358:ILE:O	2.08	0.54
1:B:441:LEU:CB	1:B:498:VAL:CG1	2.86	0.54
1:B:243:LYS:O	1:B:243:LYS:HG2	2.07	0.54
1:A:441:LEU:HD23	1:A:498:VAL:HB	1.90	0.54
1:B:492:PHE:O	1:B:492:PHE:HD1	1.90	0.54
1:B:260:SER:H	1:B:263:SER:HB3	1.72	0.54
1:B:285:ILE:HG22	1:B:329:ASN:O	2.08	0.54
1:B:232:LYS:HA	1:B:235:ILE:HG22	1.90	0.54
1:B:508:LYS:O	1:B:512:VAL:HG23	2.08	0.54
1:A:272:ILE:HG23	1:A:277:PHE:HA	1.90	0.54
1:B:285:ILE:CG1	1:B:287:ARG:CB	2.85	0.54
1:B:376:LYS:CE	1:B:376:LYS:CA	2.86	0.54
1:A:257:VAL:HG12	1:A:394:LEU:HB3	1.90	0.53
1:A:755:MSE:HE3	1:A:790:ALA:HB1	1.90	0.53
1:B:237:ILE:HD11	1:B:897:VAL:HG13	1.90	0.53
1:A:360:LEU:HB2	1:A:361:PRO:HD2	1.90	0.53
1:B:754:VAL:HA	1:B:779:PHE:HE2	1.73	0.53
1:B:255:ILE:HA	1:B:392:ILE:O	2.09	0.53
1:B:287:ARG:CD	1:B:332:VAL:HG11	2.12	0.53
1:B:754:VAL:HA	1:B:779:PHE:CE2	2.43	0.53
1:B:278:LEU:HD11	1:B:280:LYS:HG3	1.91	0.53
1:B:269:LEU:HD23	1:B:457:SER:CB	2.36	0.53
1:B:529:GLN:HG2	1:B:898:LEU:HD21	1.92	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:528:ILE:HG23	1:B:894:LEU:HD22	1.91	0.52
1:B:749:LYS:H	1:B:749:LYS:HD2	1.73	0.52
1:A:255:ILE:HD11	1:A:355:LEU:HG	1.92	0.52
1:A:400:ASP:OD1	1:A:400:ASP:N	2.41	0.52
1:B:499:SER:C	1:B:500:THR:HG23	2.34	0.52
1:B:224:ASP:N	1:B:225:ASP:OD1	2.43	0.52
1:B:259:GLY:HA2	1:B:408:ALA:HB2	1.92	0.52
1:B:308:PRO:HD2	1:B:344:ARG:O	2.10	0.52
1:B:454:GLY:H	1:B:500:THR:HG22	1.75	0.52
1:B:339:THR:CG2	1:B:340:ASP:H	2.22	0.52
1:B:318:PHE:HD1	1:B:321:ILE:HD12	1.75	0.52
1:B:387:ILE:HG22	1:B:415:VAL:HG21	1.91	0.52
1:A:294:LEU:HB3	1:A:352:ILE:HD13	1.92	0.52
1:B:454:GLY:O	1:B:500:THR:HG22	2.09	0.52
1:B:444:ARG:O	1:B:447:PRO:HD3	2.09	0.51
1:B:240:LEU:N	1:B:240:LEU:CD2	2.72	0.51
1:B:279:PRO:HG3	1:B:321:ILE:HG22	1.91	0.51
1:B:775:GLY:HA2	1:B:779:PHE:O	2.10	0.51
1:A:279:PRO:HG2	1:A:325:LEU:HD21	1.93	0.51
1:B:269:LEU:HD21	1:B:457:SER:O	2.10	0.51
1:B:453:VAL:HG21	1:B:505:LEU:HD23	1.92	0.51
1:A:631:GLN:HE21	1:A:631:GLN:HA	1.75	0.51
1:B:272:ILE:HG12	1:B:280:LYS:HG3	1.93	0.51
1:B:233:LYS:CE	1:B:233:LYS:CA	2.89	0.51
1:B:400:ASP:OD1	1:B:400:ASP:N	2.40	0.51
1:B:454:GLY:O	1:B:455:VAL:HG13	2.11	0.51
1:B:377:ARG:CG	1:B:377:ARG:NH2	2.73	0.51
1:B:671:LYS:HD2	1:B:671:LYS:N	2.26	0.51
1:B:339:THR:CG2	1:B:340:ASP:N	2.73	0.50
1:B:834:ALA:O	1:B:838:VAL:HB	2.10	0.50
1:B:254:SER:HB2	1:B:356:SER:O	2.11	0.50
1:A:617:ASP:OD1	1:A:617:ASP:N	2.44	0.50
1:B:376:LYS:HA	1:B:376:LYS:HZ3	1.73	0.50
1:B:381:GLU:OE1	1:B:381:GLU:HA	2.10	0.50
1:A:262:SER:O	1:A:266:SER:OG	2.29	0.50
1:B:434:PRO:HB3	1:B:491:GLU:HB2	1.94	0.50
1:A:264:GLY:HA2	1:A:267:SER:HB3	1.93	0.50
1:B:272:ILE:HG23	1:B:278:LEU:N	2.26	0.50
1:B:229:PHE:O	1:B:232:LYS:HG3	2.10	0.50
1:B:615:ILE:HD12	1:B:615:ILE:H	1.77	0.50
1:B:817:ASN:HB3	1:B:820:TYR:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:ILE:HA	1:A:392:ILE:O	2.12	0.49
1:A:723:VAL:HG21	1:A:824:VAL:HA	1.93	0.49
1:B:265:LYS:HA	1:B:268:VAL:CG2	2.42	0.49
1:B:458:LYS:C	1:B:458:LYS:CD	2.85	0.49
1:B:751:LEU:HA	1:B:754:VAL:HG12	1.94	0.49
1:A:289:PRO:HB2	1:A:342:PRO:HB3	1.95	0.49
1:A:704:PRO:HA	1:B:843:VAL:HG21	1.95	0.49
1:B:296:ASN:HB2	1:B:354:ASP:OD2	2.13	0.49
1:B:889:ARG:HG3	1:B:890:ARG:N	2.27	0.49
1:B:393:ILE:HG23	1:B:422:THR:HB	1.93	0.49
1:A:488:HIS:HB3	1:A:491:GLU:HG3	1.94	0.49
1:B:246:GLN:CD	1:B:247:GLY:H	2.21	0.49
1:B:376:LYS:N	1:B:376:LYS:HE2	2.28	0.49
1:B:485:PHE:HE2	1:B:500:THR:OG1	1.89	0.49
1:A:508:LYS:O	1:A:512:VAL:HG23	2.13	0.48
1:B:477:ILE:HG22	1:B:477:ILE:O	2.12	0.48
1:B:478:ASN:OD1	1:B:482:LYS:NZ	2.17	0.48
1:B:673:PRO:HD2	1:B:877:GLU:OE1	2.13	0.48
1:B:349:SER:O	1:B:352:ILE:HG13	2.13	0.48
1:A:664:LEU:HD23	1:A:676:ARG:HG3	1.96	0.48
1:B:387:ILE:O	1:B:421:ARG:NH2	2.46	0.48
1:B:593:LEU:HD21	1:B:823:GLU:HG3	1.94	0.48
1:A:254:SER:HB2	1:A:356:SER:O	2.14	0.48
1:A:616:ILE:HD13	1:A:802:LEU:HD13	1.94	0.48
1:B:279:PRO:O	1:B:280:LYS:CG	2.62	0.48
1:B:269:LEU:HD23	1:B:457:SER:HB2	1.88	0.48
1:B:478:ASN:HD21	1:B:482:LYS:NZ	1.90	0.48
1:B:742:GLU:CD	1:B:748:ARG:HE	2.20	0.48
1:A:449:LYS:C	1:A:451:GLY:H	2.20	0.48
1:B:310:LEU:N	1:B:310:LEU:CD2	2.73	0.48
1:B:639:LEU:O	1:B:642:LEU:HD23	2.14	0.48
1:B:886:ASP:HA	1:B:889:ARG:HG2	1.95	0.48
1:B:307:PHE:CD1	1:B:345:LEU:HD21	2.40	0.47
1:B:456:ILE:HD12	1:B:456:ILE:C	2.39	0.47
1:A:252:LEU:HD23	1:A:524:THR:HG21	1.95	0.47
1:A:285:ILE:HD12	1:A:287:ARG:N	2.23	0.47
1:B:278:LEU:HD13	1:B:278:LEU:C	2.39	0.47
1:B:269:LEU:HD23	1:B:457:SER:OG	2.06	0.47
1:B:483:ASN:C	1:B:483:ASN:ND2	2.73	0.47
1:A:640:THR:HG21	1:A:706:LYS:HA	1.95	0.47
1:A:714:ASN:OD1	1:A:714:ASN:N	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:491:GLU:N	1:B:491:GLU:CD	2.73	0.47
1:B:865:MSE:HB3	1:B:871:LEU:HB2	1.96	0.47
1:B:267:SER:HB2	1:B:396:ILE:CD1	2.45	0.47
1:A:596:ARG:HD2	1:A:631:GLN:HG3	1.97	0.47
1:B:278:LEU:CD2	1:B:279:PRO:O	2.57	0.47
1:B:441:LEU:CB	1:B:498:VAL:HG12	2.43	0.47
1:B:308:PRO:HG3	1:B:344:ARG:CG	2.44	0.47
1:A:607:PRO:HD3	1:A:762:ARG:HG3	1.96	0.46
1:B:472:ASN:ND2	1:B:472:ASN:O	2.47	0.46
1:A:284:MSE:SE	1:A:284:MSE:H	2.48	0.46
1:B:279:PRO:HB3	1:B:322:GLN:CG	2.45	0.46
1:B:596:ARG:HG3	1:B:635:ALA:HB2	1.97	0.46
1:B:238:ARG:CZ	1:B:356:SER:OG	2.64	0.46
1:B:377:ARG:O	1:B:380:THR:OG1	2.28	0.46
1:A:227:MSE:HA	1:A:230:ILE:HG22	1.98	0.46
1:A:599:ASN:OD1	1:A:599:ASN:N	2.48	0.46
1:A:873:LYS:O	1:A:877:GLU:HG3	2.15	0.46
1:B:285:ILE:HG12	1:B:332:VAL:HG21	1.87	0.46
1:B:270:GLU:C	1:B:273:VAL:HG22	2.40	0.46
1:B:275:HIS:CD2	1:B:275:HIS:N	2.84	0.46
1:B:474:LEU:HG	1:B:475:ALA:H	1.80	0.46
1:B:401:THR:HG22	1:B:402:ASP:O	2.16	0.45
1:B:454:GLY:O	1:B:455:VAL:CG1	2.65	0.45
1:B:454:GLY:N	1:B:500:THR:HG22	2.30	0.45
1:B:768:VAL:HG23	1:B:770:GLY:H	1.81	0.45
1:B:272:ILE:CG1	1:B:278:LEU:HD11	2.46	0.45
1:B:484:TYR:HE1	1:B:492:PHE:CZ	2.33	0.45
1:B:727:LEU:HD21	1:B:823:GLU:HG2	1.98	0.45
1:B:224:ASP:CG	1:B:227:MSE:CB	2.88	0.45
1:B:278:LEU:CD1	1:B:280:LYS:HG2	2.47	0.45
1:B:284:MSE:CG	1:B:286:THR:CG2	2.85	0.45
1:B:286:THR:HB	1:B:361:PRO:CB	2.36	0.45
1:B:576:GLN:H	1:B:576:GLN:HE21	1.60	0.45
1:A:231:THR:O	1:A:235:ILE:HG22	2.17	0.45
1:A:234:MSE:HA	1:A:237:ILE:HG22	1.97	0.45
1:A:235:ILE:HD13	1:A:356:SER:HB2	1.98	0.45
1:A:393:ILE:HG23	1:A:422:THR:HB	1.98	0.45
1:A:754:VAL:HG21	1:A:783:LEU:HD22	1.99	0.45
1:B:694:THR:HG21	1:B:845:MSE:HE3	1.98	0.45
1:A:488:HIS:HB3	1:A:491:GLU:CG	2.46	0.45
1:B:496:SER:OG	1:B:498:VAL:HG22	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:664:LEU:HB3	1:B:676:ARG:NH2	2.32	0.45
1:A:233:LYS:HE3	1:A:900:LYS:HD2	1.97	0.45
1:B:308:PRO:CG	1:B:344:ARG:HG3	2.47	0.45
1:B:426:ILE:HD11	1:B:440:ILE:CG2	2.04	0.45
1:A:355:LEU:HD23	1:A:357:LEU:HD22	1.99	0.45
1:A:705:TYR:CE1	1:A:832:LYS:HD3	2.52	0.45
1:B:454:GLY:C	1:B:455:VAL:HG13	2.42	0.45
1:B:238:ARG:NE	1:B:356:SER:OG	2.50	0.45
1:B:266:SER:HB2	1:B:427:THR:OG1	2.17	0.45
1:A:272:ILE:HD11	1:A:280:LYS:HB2	1.99	0.44
1:B:233:LYS:N	1:B:233:LYS:CE	2.80	0.44
1:B:487:SER:OG	1:B:488:HIS:CD2	2.70	0.44
1:A:296:ASN:H	1:A:354:ASP:HB3	1.82	0.44
1:A:344:ARG:H	1:A:344:ARG:HG2	1.63	0.44
1:A:530:ARG:HA	1:A:530:ARG:HD3	1.72	0.44
1:A:664:LEU:HB3	1:A:676:ARG:NH1	2.33	0.44
1:B:344:ARG:H	1:B:344:ARG:HG2	1.56	0.44
1:B:832:LYS:O	1:B:835:GLN:HG2	2.17	0.44
1:B:285:ILE:CG1	1:B:332:VAL:CG2	2.77	0.44
1:B:318:PHE:CD1	1:B:321:ILE:HD12	2.52	0.44
1:B:578:GLN:HA	1:B:838:VAL:HG21	1.99	0.44
1:A:285:ILE:HG12	1:A:329:ASN:O	2.17	0.44
1:B:246:GLN:CG	1:B:247:GLY:N	2.80	0.44
1:B:282:SER:HB2	1:B:283:ASN:H	1.63	0.44
1:B:445:GLN:C	1:B:446:TYR:CG	2.96	0.44
1:B:269:LEU:CG	1:B:457:SER:O	2.62	0.44
1:B:272:ILE:HG13	1:B:272:ILE:H	1.64	0.44
1:B:285:ILE:HG13	1:B:287:ARG:HB2	1.98	0.44
1:B:294:LEU:HB2	1:B:355:LEU:H	1.83	0.44
1:A:275:HIS:HB2	1:A:352:ILE:HG21	2.00	0.43
1:B:278:LEU:CD1	1:B:278:LEU:N	2.80	0.43
1:B:279:PRO:CG	1:B:322:GLN:HA	2.48	0.43
1:B:388:ARG:O	1:B:389:GLY:C	2.61	0.43
1:B:429:MSE:HE2	1:B:437:GLY:CA	2.34	0.43
1:B:485:PHE:CE2	1:B:492:PHE:CD1	3.04	0.43
1:B:863:GLU:O	1:B:867:ALA:HB3	2.18	0.43
1:B:270:GLU:C	1:B:270:GLU:CD	2.85	0.43
1:B:610:ARG:HA	1:B:610:ARG:NE	2.31	0.43
1:A:376:LYS:NZ	1:A:379:ILE:HD12	2.34	0.43
1:B:445:GLN:O	1:B:446:TYR:CG	2.60	0.43
1:B:233:LYS:HE2	1:B:233:LYS:CA	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:GLN:HE22	1:B:890:ARG:NH1	2.17	0.43
1:B:457:SER:O	1:B:458:LYS:HB2	2.18	0.43
1:B:269:LEU:CD2	1:B:269:LEU:C	2.86	0.43
1:B:278:LEU:HD22	1:B:280:LYS:CG	2.45	0.43
1:B:355:LEU:HD23	1:B:357:LEU:HD22	2.01	0.43
1:B:455:VAL:HG12	1:B:501:GLY:CA	2.49	0.43
1:B:492:PHE:CD1	1:B:492:PHE:O	2.70	0.43
1:B:565:PHE:HA	1:B:663:LEU:HD21	2.00	0.43
1:A:803:ARG:HA	1:A:803:ARG:HD3	1.70	0.43
1:A:251:THR:HG22	1:A:252:LEU:H	1.84	0.43
1:A:800:LEU:O	1:A:804:ILE:HG13	2.19	0.43
1:B:246:GLN:N	1:B:246:GLN:CD	2.74	0.43
1:B:853:PHE:HB3	1:B:854:PRO:HD3	2.01	0.43
1:A:507:LYS:HE3	1:A:507:LYS:HB2	1.85	0.43
1:A:837:ALA:O	1:A:841:LEU:HB2	2.17	0.43
1:B:278:LEU:CD1	1:B:280:LYS:CG	2.96	0.43
1:B:322:GLN:O	1:B:326:THR:OG1	2.14	0.43
1:B:345:LEU:HD23	1:B:345:LEU:HA	1.87	0.43
1:B:481:GLU:N	1:B:481:GLU:OE1	2.52	0.43
1:A:269:LEU:CD2	1:A:457:SER:HB2	2.49	0.43
1:A:605:LEU:HD22	1:A:606:SER:N	2.34	0.43
1:A:615:ILE:HD12	1:A:615:ILE:H	1.83	0.43
1:B:272:ILE:CG2	1:B:277:PHE:CD1	2.96	0.43
1:B:279:PRO:C	1:B:280:LYS:HG2	2.44	0.43
1:A:453:VAL:HG11	1:A:505:LEU:HB2	2.01	0.42
1:B:387:ILE:CG2	1:B:393:ILE:HD12	2.49	0.42
1:A:572:PHE:HB3	1:A:850:TYR:OH	2.19	0.42
1:B:269:LEU:CD2	1:B:457:SER:O	2.67	0.42
1:B:284:MSE:SE	1:B:284:MSE:O	2.87	0.42
1:A:528:ILE:HA	1:A:531:GLU:HG2	2.01	0.42
1:B:286:THR:CB	1:B:361:PRO:HB3	2.37	0.42
1:A:683:ALA:HB2	1:A:853:PHE:CE1	2.55	0.42
1:B:279:PRO:O	1:B:280:LYS:HG2	2.19	0.42
1:A:268:VAL:HB	1:A:280:LYS:HB3	2.02	0.42
1:A:357:LEU:HD23	1:A:357:LEU:H	1.85	0.42
1:A:744:SER:OG	1:A:786:ARG:NH2	2.51	0.42
1:B:484:TYR:CD1	1:B:484:TYR:C	2.97	0.42
1:B:255:ILE:HG12	1:B:513:LEU:HD21	2.01	0.42
1:B:574:ARG:N	1:B:575:PRO:HD2	2.33	0.42
1:B:640:THR:HG22	1:B:706:LYS:HG2	2.01	0.42
1:A:227:MSE:O	1:A:231:THR:OG1	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:GLU:HG2	1:A:277:PHE:N	2.34	0.42
1:A:387:ILE:HG22	1:A:415:VAL:HG21	2.02	0.42
1:B:297:ASP:OD1	1:B:300:ALA:HB2	2.09	0.42
1:B:496:SER:OG	1:B:498:VAL:CG2	2.68	0.42
1:A:611:GLU:N	1:A:612:PRO:HD2	2.35	0.42
1:B:285:ILE:HG22	1:B:329:ASN:CA	2.50	0.42
1:B:241:LEU:HD21	1:B:528:ILE:HD11	2.01	0.41
1:B:252:LEU:HD23	1:B:252:LEU:HA	1.89	0.41
1:B:269:LEU:HD23	1:B:270:GLU:CA	2.50	0.41
1:B:433:GLU:HA	1:B:434:PRO:HD2	1.84	0.41
1:A:244:VAL:HA	1:A:893:LEU:HD13	2.02	0.41
1:B:246:GLN:HG2	1:B:247:GLY:N	2.34	0.41
1:B:272:ILE:CG2	1:B:278:LEU:N	2.81	0.41
1:B:309:ASP:C	1:B:310:LEU:HD23	2.45	0.41
1:B:642:LEU:HD12	1:B:643:GLY:N	2.35	0.41
1:B:288:ARG:HA	1:B:289:PRO:HD3	1.79	0.41
1:B:672:HIS:HA	1:B:877:GLU:OE2	2.20	0.41
1:B:237:ILE:HD13	1:B:237:ILE:C	2.45	0.41
1:B:683:ALA:HB2	1:B:853:PHE:CE1	2.56	0.41
1:B:458:LYS:HA	1:B:458:LYS:HD2	1.97	0.41
1:B:456:ILE:O	1:B:456:ILE:HG23	2.21	0.41
1:A:269:LEU:HD11	1:A:457:SER:O	2.19	0.41
1:A:389:GLY:O	1:A:391:ASN:N	2.48	0.41
1:B:255:ILE:HG13	1:B:357:LEU:HA	2.03	0.41
1:B:270:GLU:CA	1:B:273:VAL:HG22	2.51	0.41
1:B:392:ILE:HD12	1:B:421:ARG:O	2.21	0.41
1:B:723:VAL:HG11	1:B:823:GLU:HB3	2.03	0.41
1:B:749:LYS:O	1:B:753:GLU:HG3	2.21	0.41
1:A:376:LYS:HZ2	1:A:376:LYS:HG3	1.76	0.41
1:A:423:ILE:HG22	1:A:450:LEU:HD13	2.02	0.40
1:B:455:VAL:CG1	1:B:501:GLY:H	2.19	0.40
1:B:832:LYS:O	1:B:836:THR:HG22	2.20	0.40
1:B:272:ILE:CG1	1:B:278:LEU:CD1	2.99	0.40
1:B:224:ASP:OD2	1:B:227:MSE:CB	2.69	0.40
1:B:235:ILE:HD12	1:B:235:ILE:C	2.42	0.40
1:B:307:PHE:CD1	1:B:307:PHE:N	2.90	0.40
1:B:311:GLY:O	1:B:312:LEU:HB2	2.21	0.40

All (1) 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)
1:A:630:ARG:NH1	1:B:545:GLU:OE1[5_555]	2.17	0.03

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	652/939 (69%)	627 (96%)	25 (4%)	0	100	100
1	B	652/939 (69%)	626 (96%)	26 (4%)	0	100	100
All	All	1304/1878 (69%)	1253 (96%)	51 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	564/756 (75%)	491 (87%)	73 (13%)	4	22
1	B	564/756 (75%)	465 (82%)	99 (18%)	2	12
All	All	1128/1512 (75%)	956 (85%)	172 (15%)	3	17

All (172) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	231	THR
1	A	237	ILE
1	A	244	VAL

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Mol	Chain	Res	Type
1	A	251	THR
1	A	255	ILE
1	A	266	SER
1	A	269	LEU
1	A	273	VAL
1	A	278	LEU
1	A	282	SER
1	A	283	ASN
1	A	284	MSE
1	A	285	ILE
1	A	286	THR
1	A	287	ARG
1	A	303	ASP
1	A	320	LEU
1	A	339	THR
1	A	344	ARG
1	A	346	THR
1	A	358	ILE
1	A	376	LYS
1	A	377	ARG
1	A	378	LYS
1	A	382	LEU
1	A	385	LYS
1	A	388	ARG
1	A	393	ILE
1	A	394	LEU
1	A	396	ILE
1	A	400	ASP
1	A	402	ASP
1	A	412	SER
1	A	423	ILE
1	A	430	ASP
1	A	448	LEU
1	A	458	LYS
1	A	474	LEU
1	A	479	ARG
1	A	481	GLU
1	A	483	ASN
1	A	490	THR
1	A	491	GLU
1	A	492	PHE
1	A	500	THR

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Mol	Chain	Res	Type
1	A	503	MSE
1	A	557	SER
1	A	600	ARG
1	A	602	ILE
1	A	605	LEU
1	A	610	ARG
1	A	613	ASP
1	A	615	ILE
1	A	617	ASP
1	A	618	LEU
1	A	631	GLN
1	A	632	LEU
1	A	640	THR
1	A	642	LEU
1	A	654	SER
1	A	666	LYS
1	A	690	ARG
1	A	714	ASN
1	A	727	LEU
1	A	741	LEU
1	A	803	ARG
1	A	815	LEU
1	A	817	ASN
1	A	824	VAL
1	A	838	VAL
1	A	841	LEU
1	A	873	LYS
1	A	880	LYS
1	B	225	ASP
1	B	227	MSE
1	B	228	MSE
1	B	229	PHE
1	B	230	ILE
1	B	233	LYS
1	B	235	ILE
1	B	237	ILE
1	B	240	LEU
1	B	241	LEU
1	B	243	LYS
1	B	244	VAL
1	B	255	ILE
1	B	263	SER

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Mol	Chain	Res	Type
1	B	266	SER
1	B	268	VAL
1	B	269	LEU
1	B	272	ILE
1	B	278	LEU
1	B	282	SER
1	B	283	ASN
1	B	284	MSE
1	B	285	ILE
1	B	303	ASP
1	B	310	LEU
1	B	320	LEU
1	B	344	ARG
1	B	346	THR
1	B	351	ASN
1	B	354	ASP
1	B	358	ILE
1	B	360	LEU
1	B	363	TYR
1	B	375	LEU
1	B	376	LYS
1	B	377	ARG
1	B	378	LYS
1	B	382	LEU
1	B	383	CYS
1	B	385	LYS
1	B	388	ARG
1	B	393	ILE
1	B	394	LEU
1	B	396	ILE
1	B	400	ASP
1	B	402	ASP
1	B	407	THR
1	B	412	SER
1	B	423	ILE
1	B	430	ASP
1	B	434	PRO
1	B	448	LEU
1	B	450	LEU
1	B	456	ILE
1	B	457	SER
1	B	458	LYS

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Mol	Chain	Res	Type
1	B	474	LEU
1	B	479	ARG
1	B	481	GLU
1	B	483	ASN
1	B	491	GLU
1	B	498	VAL
1	B	499	SER
1	B	505	LEU
1	B	507	LYS
1	B	513	LEU
1	B	515	GLN
1	B	516	GLN
1	B	546	GLN
1	B	560	ASP
1	B	576	GLN
1	B	586	ASP
1	B	610	ARG
1	B	615	ILE
1	B	617	ASP
1	B	631	GLN
1	B	632	LEU
1	B	640	THR
1	B	642	LEU
1	B	647	LEU
1	B	654	SER
1	B	657	GLN
1	B	671	LYS
1	B	703	LYS
1	B	714	ASN
1	B	727	LEU
1	B	739	LYS
1	B	749	LYS
1	B	768	VAL
1	B	784	LEU
1	B	802	LEU
1	B	815	LEU
1	B	836	THR
1	B	838	VAL
1	B	839	LEU
1	B	841	LEU
1	B	871	LEU
1	B	893	LEU

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Mol	Chain	Res	Type
1	B	903	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	658	GLN
1	A	712	GLN
1	B	242	GLN
1	B	261	GLN
1	B	275	HIS
1	B	472	ASN
1	B	478	ASN
1	B	488	HIS
1	B	515	GLN
1	B	576	GLN
1	B	657	GLN
1	B	659	HIS
1	B	811	GLN
1	B	847	ASN
1	B	864	HIS
1	B	866	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](#)

2 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	$\# Z > 2$
2	EDO	A	1001	-	3,3,3	0.42	0	2,2,2	0.38	0
2	EDO	B	1001	-	3,3,3	0.43	0	2,2,2	0.38	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
2	EDO	A	1001	-	-	0/1/1/1	-
2	EDO	B	1001	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	253:PRO	C	254:SER	N	1.13

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	648/939 (69%)	0.31	32 (4%) 35 20	64, 116, 190, 232	2 (0%)
1	B	648/939 (69%)	0.45	43 (6%) 24 15	64, 116, 338, 374	1 (0%)
All	All	1296/1878 (69%)	0.38	75 (5%) 29 17	64, 116, 320, 374	3 (0%)

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	270	GLU	7.5
1	B	458	LYS	6.1
1	A	458	LYS	5.1
1	A	487	SER	4.8
1	B	273	VAL	4.8
1	A	265	LYS	4.6
1	B	453	VAL	4.6
1	B	769	GLU	4.5
1	A	270	GLU	4.3
1	A	430	ASP	4.1
1	A	375	LEU	4.1
1	B	375	LEU	4.1
1	B	267	SER	4.0
1	B	452	TYR	3.7
1	B	388	ARG	3.7
1	B	265	LYS	3.7
1	B	474	LEU	3.7
1	B	364	ILE	3.5
1	B	428	LYS	3.4
1	B	502	VAL	3.3
1	B	277	PHE	3.2
1	B	274	GLY	3.1
1	A	612	PRO	3.0
1	B	271	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	643	GLY	2.9
1	B	310	LEU	2.8
1	A	488	HIS	2.8
1	B	353	PRO	2.8
1	A	273	VAL	2.8
1	B	471	GLY	2.8
1	A	474	LEU	2.8
1	B	278	LEU	2.7
1	A	611	GLU	2.7
1	A	275	HIS	2.7
1	B	457	SER	2.7
1	A	280	LYS	2.6
1	B	424	GLY	2.6
1	B	473	LEU	2.6
1	B	347	ILE	2.6
1	A	264	GLY	2.6
1	A	286	THR	2.6
1	A	376	LYS	2.6
1	A	246	GLN	2.6
1	A	502	VAL	2.5
1	B	275	HIS	2.5
1	A	604	ASP	2.5
1	B	455	VAL	2.4
1	B	456	ILE	2.4
1	A	263	SER	2.4
1	A	473	LEU	2.3
1	B	425	VAL	2.3
1	B	447	PRO	2.3
1	A	312	LEU	2.3
1	A	784	LEU	2.2
1	B	417	PRO	2.2
1	B	319	SER	2.2
1	B	386	TYR	2.2
1	B	435	GLU	2.2
1	A	747	GLY	2.2
1	B	291	GLU	2.2
1	B	409	LEU	2.2
1	B	268	VAL	2.1
1	A	405	ASN	2.1
1	A	768	VAL	2.1
1	B	294	LEU	2.1
1	A	359	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	428	LYS	2.0
1	A	481	GLU	2.0
1	B	381	GLU	2.0
1	A	485	PHE	2.0
1	A	471	GLY	2.0
1	A	501	GLY	2.0
1	B	280	LYS	2.0
1	B	387	ILE	2.0
1	B	418	ARG	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, 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($\text{\AA}^2$)	Q<0.9
2	EDO	B	1001	4/4	0.58	0.29	97,97,97,97	0
2	EDO	A	1001	4/4	0.81	0.26	105,105,105,105	0

6.5 Other polymers [i](#)

There are no such residues in this entry.