



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 03:30 am GMT

PDB ID : 1XHX
Title : Phi29 DNA Polymerase, orthorhombic crystal form
Authors : Kamtekar, S.; Berman, A.J.; Wang, J.; Lazaro, J.M.; de Vega, M.; Blanco, L.; Salas, M.; Steitz, T.A.
Deposited on : 2004-09-21
Resolution : 2.35 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

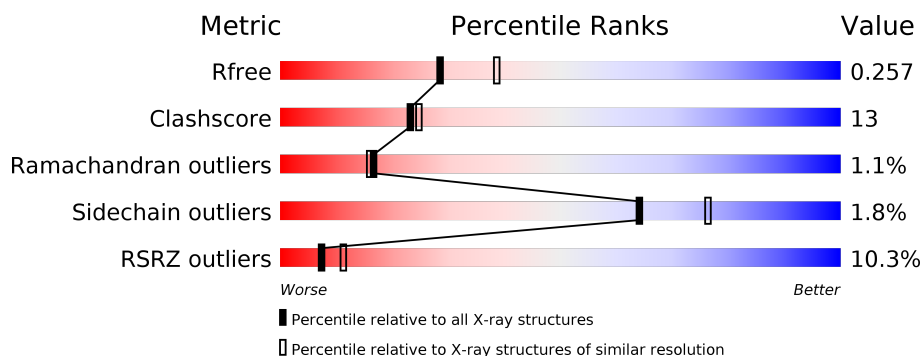
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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}	100719	1522 (2.38-2.34)
Clashscore	112137	1626 (2.38-2.34)
Ramachandran outliers	110173	1605 (2.38-2.34)
Sidechain outliers	110143	1606 (2.38-2.34)
RSRZ outliers	101464	1528 (2.38-2.34)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	575	<div> <div>14%</div> <div> <div></div> <div>73%</div> <div>25%</div> <div>..</div> </div> </div>
1	B	575	<div> <div>11%</div> <div> <div></div> <div>72%</div> <div>26%</div> <div>..</div> </div> </div>
1	C	575	<div> <div>11%</div> <div> <div></div> <div>73%</div> <div>25%</div> <div>..</div> </div> </div>
1	D	575	<div> <div>5%</div> <div> <div></div> <div>79%</div> <div>19%</div> <div>..</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MG	C	5000	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 20193 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 DNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	571	Total	C	N	O	S	0	0	0
			4668	3041	754	852	21			
1	B	571	Total	C	N	O	S	0	0	0
			4668	3041	754	852	21			
1	C	571	Total	C	N	O	S	0	0	0
			4668	3041	754	852	21			
1	D	571	Total	C	N	O	S	0	0	0
			4668	3041	754	852	21			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	ALA	ASP	ENGINEERED	UNP P03680
A	66	ALA	ASP	ENGINEERED	UNP P03680
B	12	ALA	ASP	ENGINEERED	UNP P03680
B	66	ALA	ASP	ENGINEERED	UNP P03680
C	12	ALA	ASP	ENGINEERED	UNP P03680
C	66	ALA	ASP	ENGINEERED	UNP P03680
D	12	ALA	ASP	ENGINEERED	UNP P03680
D	66	ALA	ASP	ENGINEERED	UNP P03680

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	2	Total	Mg	0	0
			2	2		

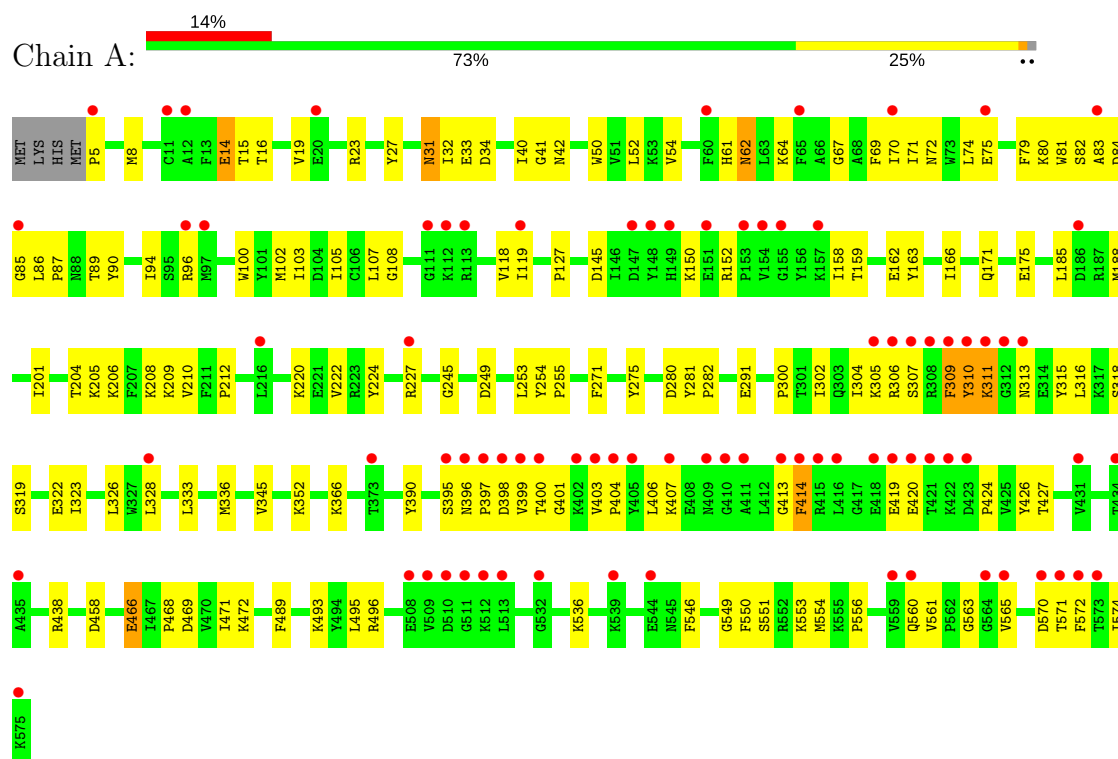
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	295	Total	O	0	0
			295	295		
4	B	388	Total	O	0	0
			388	388		
4	C	382	Total	O	0	0
			382	382		
4	D	444	Total	O	0	0
			444	444		

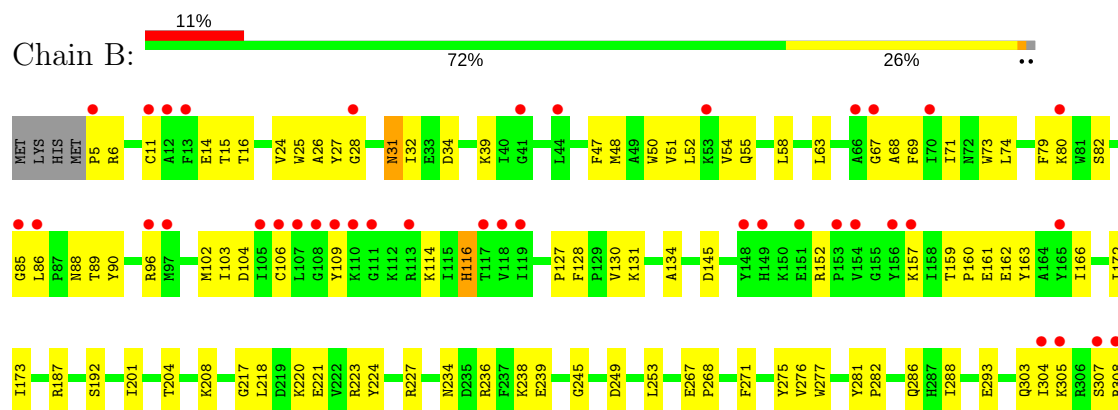
3 Residue-property plots [i](#)

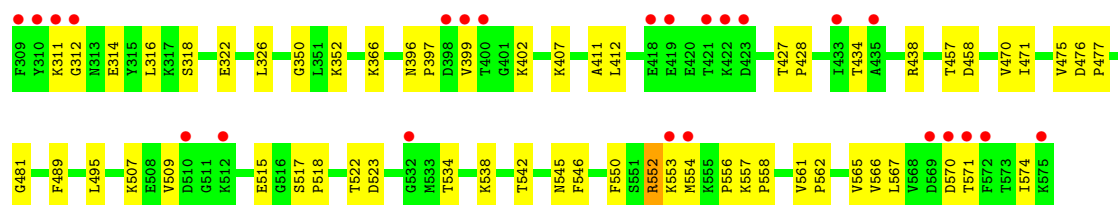
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: DNA polymerase

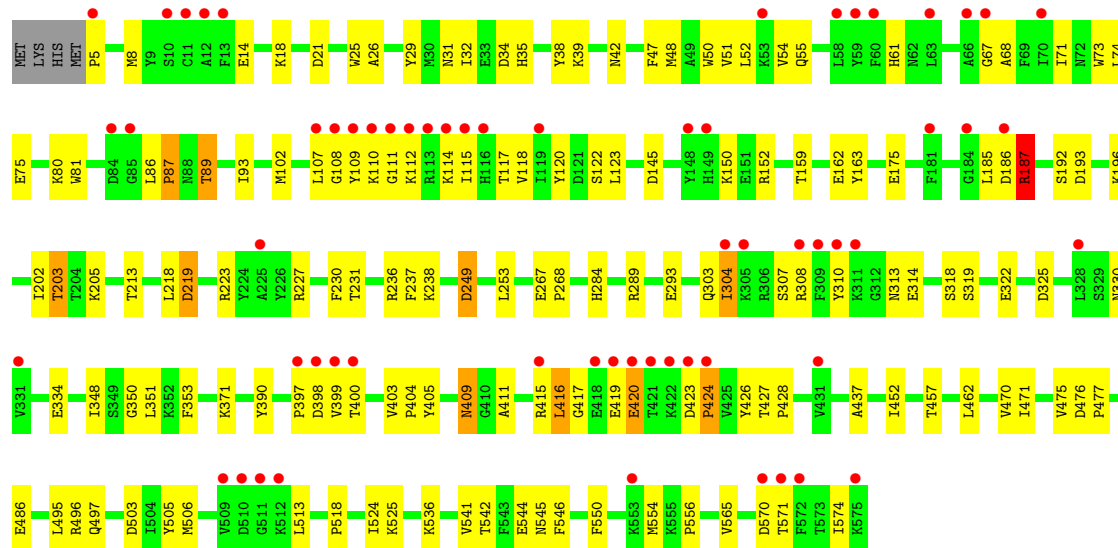


• Molecule 1: DNA polymerase

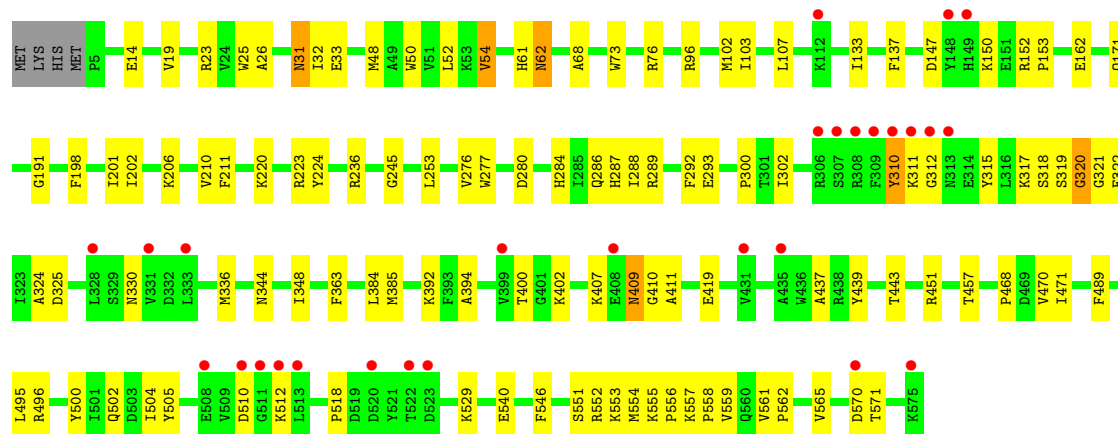
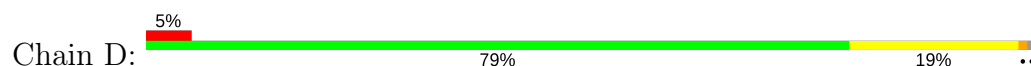




● Molecule 1: DNA polymerase



● Molecule 1: DNA polymerase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	96.26Å 149.91Å 199.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.96 – 2.35 30.72 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.7 (19.96-2.35) 99.8 (30.72-2.35)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 2.36Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.206 , 0.257 0.207 , 0.257	Depositor DCC
R_{free} test set	11990 reflections (10.01%)	DCC
Wilson B-factor (Å ²)	42.7	Xtriage
Anisotropy	0.251	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 47.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	20193	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% 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: MG, SO4

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	0.35	0/4788	0.65	3/6459 (0.0%)
1	B	0.36	0/4788	0.62	0/6459
1	C	0.36	0/4788	0.61	0/6459
1	D	0.38	0/4788	0.62	0/6459
All	All	0.36	0/19152	0.63	3/25836 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	5	PRO	CA-N-CD	-13.35	92.81	111.50
1	A	309	PHE	CA-CB-CG	-6.95	97.21	113.90
1	A	309	PHE	CA-C-N	-5.65	104.77	117.20

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	4668	0	4676	134	0
1	B	4668	0	4676	116	0
1	C	4668	0	4676	141	0
1	D	4668	0	4676	97	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	10	0	0	0	0
3	C	2	0	0	0	0
4	A	295	0	0	9	0
4	B	388	0	0	4	0
4	C	382	0	0	12	0
4	D	444	0	0	7	0
All	All	20193	0	18704	478	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 13.

All (478) 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:310:TYR:OH	1:A:322:GLU:HG3	1.37	1.23
1:C:223:ARG:NH2	1:C:424:PRO:HG2	1.70	1.06
1:C:110:LYS:HG2	1:C:115:ILE:HD11	1.36	1.04
1:B:89:THR:HG22	1:B:90:TYR:H	1.22	1.03
1:A:75:GLU:HB3	1:A:406:LEU:HD11	1.45	0.98
1:C:52:LEU:HD22	1:C:107:LEU:HD21	1.46	0.98
1:A:86:LEU:O	1:A:89:THR:HB	1.69	0.91
1:C:223:ARG:HH22	1:C:424:PRO:HG2	1.25	0.91
1:A:310:TYR:O	1:A:311:LYS:HB2	1.72	0.87
1:C:110:LYS:CG	1:C:115:ILE:HD11	2.05	0.85
1:B:89:THR:HG22	1:B:90:TYR:N	1.91	0.85
1:D:96:ARG:O	1:D:402:LYS:HE3	1.76	0.85
1:A:82:SER:HB3	1:A:89:THR:HG23	1.58	0.85
1:B:5:PRO:HG3	1:C:5:PRO:HG3	1.58	0.84
1:A:52:LEU:HD22	1:A:107:LEU:HD21	1.60	0.83
1:B:82:SER:OG	1:B:89:THR:HG21	1.78	0.83
1:A:310:TYR:HH	1:A:322:GLU:HG3	1.43	0.81
1:A:82:SER:HB3	1:A:89:THR:CG2	2.10	0.81
1:D:289:ARG:HG3	1:D:348:ILE:HD11	1.61	0.81
1:B:80:LYS:O	1:B:89:THR:HG23	1.79	0.81
1:C:87:PRO:HG3	1:C:108:GLY:HA2	1.60	0.81
1:A:75:GLU:HG3	1:A:406:LEU:HD21	1.63	0.80
1:A:81:TRP:CH2	1:A:83:ALA:HB2	2.18	0.79
1:D:363:PHE:CZ	1:D:385:MET:HE3	2.17	0.79
1:D:52:LEU:O	1:D:107:LEU:HD11	1.83	0.79
1:D:540:GLU:HB3	1:D:552:ARG:HH11	1.49	0.77
1:D:561:VAL:HG12	1:D:562:PRO:HD2	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:THR:OG1	1:B:162:GLU:HG3	1.84	0.76
1:B:407:LYS:HB2	1:B:411:ALA:O	1.86	0.76
1:C:202:ILE:O	1:C:203:THR:HB	1.84	0.75
1:A:220:LYS:HE2	1:A:224:TYR:OH	1.85	0.75
1:C:31:ASN:HD22	1:C:34:ASP:N	1.83	0.75
1:B:114:LYS:HE3	1:B:116:HIS:HD2	1.51	0.75
1:D:14:GLU:HB2	1:D:26:ALA:HB3	1.69	0.75
1:B:227:ARG:NH2	1:B:305:LYS:HE2	2.02	0.74
1:C:150:LYS:HD3	1:C:152:ARG:NH1	2.02	0.74
1:C:50:TRP:CE2	1:C:54:VAL:HG11	2.23	0.73
1:D:496:ARG:HG3	1:D:496:ARG:HH11	1.51	0.73
1:D:540:GLU:HB3	1:D:552:ARG:NH1	2.03	0.73
1:C:31:ASN:HD22	1:C:34:ASP:H	1.35	0.72
1:A:310:TYR:OH	1:A:322:GLU:CG	2.30	0.72
1:C:29:TYR:CZ	1:C:39:LYS:HB3	2.25	0.71
1:C:304:ILE:HG22	1:D:344:ASN:HA	1.71	0.71
1:C:159:THR:OG1	1:C:162:GLU:HG3	1.91	0.71
1:A:205:LYS:HE2	1:A:209:LYS:NZ	2.05	0.71
1:B:89:THR:CG2	1:B:90:TYR:H	2.00	0.70
1:A:64:LYS:HG3	1:A:100:TRP:NE1	2.07	0.70
1:B:522:THR:HG22	1:B:523:ASP:OD1	1.92	0.69
1:C:409:ASN:H	1:C:409:ASN:HD22	1.41	0.69
1:C:307:SER:HB3	1:C:310:TYR:CD1	2.27	0.69
1:A:310:TYR:CZ	1:A:322:GLU:HG3	2.27	0.69
1:C:14:GLU:HB2	1:C:26:ALA:HB3	1.74	0.69
1:C:150:LYS:HD3	1:C:152:ARG:HH12	1.56	0.69
1:A:227:ARG:HH22	1:A:305:LYS:HG3	1.58	0.68
1:B:14:GLU:HB2	1:B:26:ALA:HB3	1.76	0.68
1:A:74:LEU:O	1:A:79:PHE:HB2	1.95	0.68
1:D:551:SER:O	1:D:552:ARG:HG3	1.93	0.68
1:C:397:PRO:O	1:C:399:VAL:HG23	1.94	0.67
1:C:542:THR:OG1	1:C:545:ASN:HB3	1.95	0.67
1:D:554:MET:O	1:D:556:PRO:HD3	1.95	0.66
1:B:481:GLY:HA3	4:B:849:HOH:O	1.96	0.66
1:C:8:MET:HB3	1:C:32:ILE:HD12	1.77	0.66
1:C:236:ARG:HH21	1:C:237:PHE:HZ	1.42	0.66
1:A:496:ARG:HG3	1:A:496:ARG:HH11	1.60	0.65
1:A:560:GLN:HG2	1:A:565:VAL:HG22	1.77	0.65
1:A:310:TYR:O	1:A:311:LYS:CB	2.44	0.65
1:A:306:ARG:O	1:A:307:SER:OG	2.13	0.65
1:B:5:PRO:HG3	1:C:5:PRO:CG	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:496:ARG:HG2	1:C:496:ARG:HH11	1.60	0.65
1:D:310:TYR:N	1:D:310:TYR:CD2	2.61	0.65
1:D:302:ILE:HD11	1:D:336:MET:SD	2.36	0.65
1:B:71:ILE:HB	1:B:412:LEU:HD11	1.78	0.65
1:D:363:PHE:HZ	1:D:385:MET:HE3	1.61	0.65
1:B:545:ASN:HD21	1:B:550:PHE:HE1	1.44	0.64
1:B:293:GLU:OE2	1:B:318:SER:HB2	1.97	0.64
1:C:231:THR:HB	1:C:313:ASN:HD22	1.62	0.64
1:C:452:ILE:HA	1:C:462:LEU:HD23	1.78	0.64
1:C:403:VAL:HG23	1:C:417:GLY:HA3	1.80	0.64
1:A:150:LYS:O	1:A:152:ARG:HG3	1.98	0.64
1:C:223:ARG:HH22	1:C:424:PRO:CG	2.05	0.63
1:C:185:LEU:HD22	1:C:193:ASP:HB3	1.80	0.63
1:A:50:TRP:CE2	1:A:54:VAL:HG11	2.33	0.63
1:C:48:MET:HE2	1:C:48:MET:HA	1.81	0.63
1:A:553:LYS:HG2	1:A:571:THR:OG1	1.98	0.63
1:D:505:TYR:CE1	1:D:518:PRO:HG3	2.33	0.63
1:C:48:MET:HE1	1:C:51:VAL:HG21	1.81	0.63
1:A:345:VAL:HB	1:B:322:GLU:HG3	1.79	0.63
1:D:220:LYS:HE2	1:D:224:TYR:OH	1.99	0.62
1:C:541:VAL:HA	1:C:545:ASN:ND2	2.14	0.62
1:C:470:VAL:HG23	1:C:471:ILE:HG23	1.82	0.62
1:D:280:ASP:HB2	4:D:3210:HOH:O	1.99	0.62
1:B:471:ILE:O	1:B:475:VAL:HG23	2.00	0.62
1:A:67:GLY:O	1:A:71:ILE:HG12	1.99	0.62
1:B:220:LYS:HE2	1:B:224:TYR:OH	1.99	0.62
1:B:561:VAL:HG13	1:B:562:PRO:HD2	1.81	0.62
1:C:399:VAL:HG13	1:C:420:GLU:O	2.00	0.61
1:C:554:MET:O	1:C:556:PRO:HD3	1.99	0.61
1:C:61:HIS:O	1:C:123:LEU:HB2	2.01	0.61
1:B:5:PRO:CG	1:C:5:PRO:HG3	2.31	0.61
1:A:323:ILE:HG13	1:B:307:SER:OG	2.00	0.61
1:D:96:ARG:HE	1:D:400:THR:HB	1.65	0.61
1:A:554:MET:O	1:A:556:PRO:HD3	2.01	0.60
1:C:293:GLU:OE2	1:C:318:SER:HB2	2.01	0.60
1:B:399:VAL:O	1:B:399:VAL:HG12	2.01	0.60
1:A:87:PRO:HG3	1:A:108:GLY:HA2	1.82	0.60
1:A:74:LEU:HD21	1:A:105:ILE:HD13	1.83	0.60
1:B:187:ARG:HD2	4:B:747:HOH:O	2.02	0.60
1:A:291:GLU:HG3	1:A:323:ILE:HD13	1.83	0.60
1:A:94:ILE:O	1:A:401:GLY:HA3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:TRP:NE1	1:B:54:VAL:HG11	2.17	0.60
1:A:31:ASN:HD22	1:A:31:ASN:C	2.05	0.60
1:D:31:ASN:ND2	1:D:33:GLU:H	1.99	0.59
1:D:198:PHE:O	1:D:201:ILE:HG22	2.03	0.59
1:B:545:ASN:ND2	1:B:550:PHE:HE1	2.00	0.59
1:C:471:ILE:O	1:C:475:VAL:HG23	2.02	0.59
1:A:466:GLU:H	1:A:466:GLU:CD	2.05	0.59
1:D:19:VAL:O	1:D:561:VAL:HG11	2.03	0.58
1:A:31:ASN:HD22	1:A:32:ILE:N	2.00	0.58
1:B:55:GLN:HA	1:B:116:HIS:O	2.03	0.58
1:D:31:ASN:HD22	1:D:33:GLU:H	1.52	0.58
1:C:187:ARG:N	1:C:187:ARG:HD2	2.18	0.58
1:A:31:ASN:ND2	1:A:33:GLU:H	2.02	0.58
1:B:227:ARG:HD2	1:B:303:GLN:OE1	2.04	0.58
1:A:400:THR:OG1	1:A:419:GLU:HA	2.04	0.58
1:A:15:THR:HG22	1:A:16:THR:N	2.18	0.58
1:B:85:GLY:O	1:B:109:TYR:HE1	1.87	0.57
1:C:18:LYS:HB2	1:C:21:ASP:O	2.04	0.57
1:D:489:PHE:HB3	1:D:504:ILE:HD13	1.86	0.57
1:B:162:GLU:O	1:B:166:ILE:HG13	2.04	0.57
1:D:502:GLN:OE1	1:D:504:ILE:HD11	2.04	0.57
1:C:495:LEU:O	1:C:496:ARG:HG2	2.03	0.57
1:A:15:THR:CG2	1:A:16:THR:N	2.66	0.57
1:C:223:ARG:CZ	1:C:397:PRO:HG2	2.35	0.57
1:D:553:LYS:HA	1:D:571:THR:HA	1.84	0.57
1:D:561:VAL:HG12	1:D:562:PRO:CD	2.35	0.57
1:D:496:ARG:HG3	1:D:496:ARG:NH1	2.20	0.57
1:A:162:GLU:O	1:A:166:ILE:HG13	2.05	0.57
1:C:238:LYS:HE3	1:C:496:ARG:NH1	2.19	0.57
1:A:281:TYR:HB3	1:A:352:LYS:HB3	1.85	0.56
1:B:50:TRP:CE2	1:B:54:VAL:HG11	2.41	0.56
1:D:31:ASN:C	1:D:31:ASN:HD22	2.08	0.56
1:D:253:LEU:HD21	1:D:437:ALA:HB1	1.85	0.56
1:C:399:VAL:HG12	1:C:419:GLU:HB3	1.88	0.56
1:B:67:GLY:O	1:B:71:ILE:HG12	2.06	0.56
1:C:109:TYR:CE2	1:C:114:LYS:HG2	2.40	0.56
1:A:313:ASN:HB3	4:A:749:HOH:O	2.05	0.56
1:B:470:VAL:HG13	1:B:471:ILE:HG23	1.87	0.56
1:A:469:ASP:HA	1:A:472:LYS:HG3	1.86	0.55
1:C:310:TYR:HE1	1:D:289:ARG:HD3	1.71	0.55
1:C:218:LEU:HD12	4:C:5046:HOH:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:223:ARG:NH2	1:C:397:PRO:HG2	2.22	0.54
1:A:8:MET:HB3	1:A:32:ILE:HD12	1.89	0.54
1:B:106:CYS:HA	1:B:116:HIS:HB3	1.89	0.54
1:B:234:ASN:OD1	1:B:236:ARG:HG2	2.07	0.54
1:B:31:ASN:HD22	1:B:32:ILE:N	2.06	0.54
1:B:550:PHE:HB3	1:B:574:ILE:HD12	1.89	0.54
1:D:287:HIS:HE1	1:D:325:ASP:OD1	1.89	0.54
1:A:14:GLU:HA	1:A:14:GLU:OE1	2.08	0.54
1:C:231:THR:HB	1:C:313:ASN:ND2	2.22	0.54
1:B:553:LYS:HA	1:B:571:THR:HA	1.90	0.54
1:A:245:GLY:HA3	1:A:489:PHE:CZ	2.43	0.54
1:A:205:LYS:HE2	1:A:209:LYS:HZ2	1.72	0.54
1:B:187:ARG:HB3	1:B:192:SER:HB2	1.90	0.54
1:C:61:HIS:HA	1:C:122:SER:OG	2.08	0.54
1:C:230:PHE:HA	4:C:5269:HOH:O	2.08	0.54
1:B:161:GLU:CD	1:B:161:GLU:H	2.10	0.53
1:B:427:THR:OG1	1:B:428:PRO:HD3	2.09	0.53
1:B:253:LEU:HD22	1:B:458:ASP:HB3	1.89	0.53
1:A:16:THR:HA	4:A:579:HOH:O	2.08	0.53
1:C:75:GLU:OE1	1:C:80:LYS:HA	2.08	0.53
1:A:302:ILE:HD11	1:A:336:MET:HG3	1.90	0.53
1:A:75:GLU:CG	1:A:406:LEU:HD21	2.38	0.53
1:B:114:LYS:HE3	1:B:116:HIS:CD2	2.38	0.53
1:B:134:ALA:HB2	1:B:172:ILE:HD13	1.91	0.53
1:B:534:THR:O	1:B:538:LYS:HG3	2.08	0.53
1:C:496:ARG:HG2	1:C:496:ARG:NH1	2.24	0.53
1:C:81:TRP:CD1	1:C:404:PRO:HD2	2.44	0.53
1:C:231:THR:HG22	1:C:497:GLN:HB3	1.91	0.53
1:D:171:GLN:NE2	4:D:3064:HOH:O	2.42	0.53
1:A:81:TRP:HH2	1:A:83:ALA:HB2	1.68	0.53
1:A:210:VAL:O	1:A:212:PRO:HD3	2.09	0.53
1:C:203:THR:HG22	1:C:205:LYS:H	1.73	0.53
1:D:409:ASN:N	1:D:409:ASN:HD22	2.06	0.52
1:A:52:LEU:CD2	1:A:107:LEU:HD21	2.37	0.52
1:A:205:LYS:HE2	1:A:209:LYS:HZ1	1.74	0.52
1:B:542:THR:H	1:B:545:ASN:HB3	1.74	0.52
1:C:238:LYS:HE3	1:C:496:ARG:HH12	1.73	0.52
1:A:75:GLU:HG3	1:A:406:LEU:CD2	2.38	0.52
1:A:253:LEU:HD22	1:A:458:ASP:HB3	1.92	0.52
1:D:201:ILE:HG23	1:D:202:ILE:HG23	1.91	0.52
1:D:50:TRP:O	1:D:54:VAL:HG22	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:ILE:HG12	1:A:316:LEU:CD1	2.40	0.51
1:A:69:PHE:HD1	1:A:69:PHE:H	1.58	0.51
1:C:505:TYR:CE1	1:C:518:PRO:HG3	2.46	0.51
1:D:310:TYR:HE1	4:D:3133:HOH:O	1.93	0.51
1:B:245:GLY:HA3	1:B:489:PHE:CZ	2.45	0.51
1:C:202:ILE:O	1:C:203:THR:CB	2.58	0.51
1:D:245:GLY:HA3	1:D:489:PHE:CZ	2.46	0.51
1:D:561:VAL:CG1	1:D:562:PRO:HD2	2.37	0.51
1:A:70:ILE:HD13	1:A:119:ILE:HD13	1.92	0.51
1:B:47:PHE:O	1:B:51:VAL:HG23	2.10	0.51
1:C:409:ASN:ND2	1:C:409:ASN:H	2.07	0.51
1:A:468:PRO:HD2	1:A:471:ILE:HD11	1.93	0.51
1:A:84:ASP:HB2	4:A:593:HOH:O	2.11	0.51
1:B:50:TRP:NE1	1:B:54:VAL:CG1	2.74	0.51
1:C:249:ASP:HB2	1:C:486:GLU:HG2	1.92	0.51
1:C:570:ASP:OD1	1:C:571:THR:N	2.44	0.51
1:D:470:VAL:HG23	1:D:471:ILE:HG23	1.92	0.51
1:A:15:THR:HG21	1:A:69:PHE:HZ	1.76	0.51
1:B:102:MET:HG2	1:B:103:ILE:N	2.25	0.51
4:C:5052:HOH:O	1:D:293:GLU:HG3	2.11	0.51
1:B:96:ARG:O	1:B:402:LYS:HE3	2.11	0.51
1:D:570:ASP:OD1	1:D:571:THR:N	2.34	0.51
1:A:281:TYR:N	1:A:282:PRO:HD3	2.26	0.50
1:B:304:ILE:HD12	1:B:314:GLU:CD	2.32	0.50
1:B:6:ARG:NH1	1:B:116:HIS:HE1	2.09	0.50
1:B:227:ARG:O	1:B:434:THR:HG21	2.12	0.50
1:C:330:ASN:O	1:C:334:GLU:HG2	2.11	0.50
1:A:40:ILE:HD12	1:A:163:TYR:CD1	2.47	0.50
1:B:90:TYR:HA	1:B:104:ASP:O	2.12	0.50
1:C:80:LYS:O	1:C:89:THR:OG1	2.27	0.50
1:C:550:PHE:HB3	1:C:574:ILE:HD12	1.93	0.50
1:A:40:ILE:HD12	1:A:163:TYR:CE1	2.47	0.50
1:A:19:VAL:HG13	1:A:561:VAL:HG11	1.94	0.50
1:A:72:ASN:ND2	1:A:563:GLY:H	2.09	0.50
1:D:553:LYS:HA	1:D:570:ASP:O	2.11	0.50
1:A:495:LEU:O	1:A:496:ARG:HG3	2.11	0.50
1:C:187:ARG:NH1	1:C:187:ARG:HG3	2.26	0.50
1:A:536:LYS:HE2	1:A:554:MET:CE	2.42	0.50
1:C:68:ALA:CB	1:C:565:VAL:HG23	2.41	0.50
1:A:224:TYR:CD2	1:A:305:LYS:NZ	2.80	0.49
1:B:495:LEU:HG	1:B:546:PHE:CE2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:LEU:O	1:B:89:THR:HB	2.12	0.49
1:A:42:ASN:HB2	4:A:585:HOH:O	2.11	0.49
1:A:553:LYS:HA	1:A:571:THR:HA	1.93	0.49
1:C:51:VAL:HG13	1:C:117:THR:HG21	1.93	0.49
1:B:281:TYR:HB3	1:B:352:LYS:HB3	1.93	0.49
1:B:238:LYS:HG2	1:B:239:GLU:HG3	1.94	0.49
1:B:271:PHE:CZ	1:B:350:GLY:HA3	2.48	0.49
1:C:86:LEU:O	1:C:89:THR:HG22	2.12	0.49
1:A:304:ILE:HG12	1:A:316:LEU:HD11	1.93	0.49
1:D:300:PRO:HB2	1:D:315:TYR:HB3	1.94	0.49
1:A:27:TYR:CE2	1:A:41:GLY:HA3	2.48	0.49
1:A:399:VAL:O	1:A:420:GLU:HB2	2.13	0.49
1:B:82:SER:CB	1:B:89:THR:HG21	2.42	0.49
1:C:39:LYS:NZ	4:C:5011:HOH:O	2.45	0.49
1:D:223:ARG:NH1	4:D:3081:HOH:O	2.44	0.49
1:C:55:GLN:NE2	1:C:115:ILE:HG23	2.28	0.49
1:D:286:GLN:HG3	1:D:288:ILE:HG23	1.94	0.49
1:D:302:ILE:HD11	1:D:336:MET:HG3	1.93	0.49
1:B:15:THR:HG22	1:B:24:VAL:HA	1.93	0.49
1:B:85:GLY:O	1:B:109:TYR:CE1	2.66	0.48
1:C:400:THR:HG21	1:C:416:LEU:HD22	1.95	0.48
1:A:201:ILE:HD11	1:A:366:LYS:CD	2.44	0.48
1:A:254:TYR:HB2	1:A:255:PRO:HD3	1.96	0.48
1:C:223:ARG:HH11	1:C:223:ARG:HG2	1.79	0.48
1:C:289:ARG:HD3	1:C:325:ASP:OD1	2.14	0.48
1:D:147:ASP:OD2	1:D:150:LYS:HB2	2.14	0.48
1:A:15:THR:HG22	1:A:16:THR:O	2.13	0.48
1:A:398:ASP:O	1:A:398:ASP:OD1	2.30	0.48
1:D:293:GLU:OE2	1:D:318:SER:HB2	2.14	0.48
1:B:286:GLN:HG3	1:B:288:ILE:CG2	2.44	0.48
1:D:559:VAL:O	1:D:561:VAL:HG23	2.14	0.48
1:A:100:TRP:CD1	1:A:100:TRP:N	2.80	0.48
1:A:159:THR:OG1	1:A:162:GLU:HG3	2.14	0.48
1:A:227:ARG:HH12	1:A:305:LYS:HA	1.79	0.48
1:A:15:THR:HG21	1:A:69:PHE:CZ	2.49	0.48
1:B:227:ARG:HH11	1:B:227:ARG:HG2	1.79	0.47
1:A:102:MET:HG3	1:A:118:VAL:CG1	2.44	0.47
1:B:160:PRO:O	1:B:163:TYR:HB3	2.14	0.47
1:B:5:PRO:HG3	1:C:5:PRO:CB	2.44	0.47
1:D:495:LEU:O	1:D:496:ARG:HG3	2.14	0.47
1:C:52:LEU:HB3	1:C:107:LEU:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:500:TYR:CZ	1:D:529:LYS:HG3	2.49	0.47
1:D:31:ASN:HD22	1:D:32:ILE:N	2.13	0.47
1:A:74:LEU:HD11	1:A:105:ILE:HD11	1.96	0.47
1:B:557:LYS:HB3	1:B:570:ASP:OD2	2.14	0.47
1:C:308:ARG:HH11	1:C:308:ARG:HG3	1.80	0.47
1:A:319:SER:HB2	1:A:322:GLU:O	2.14	0.47
1:B:304:ILE:HG12	1:B:316:LEU:HD11	1.97	0.47
1:B:74:LEU:O	1:B:79:PHE:HB2	2.15	0.47
1:C:350:GLY:O	1:C:351:LEU:HD23	2.14	0.47
1:B:31:ASN:C	1:B:31:ASN:HD22	2.17	0.47
1:C:541:VAL:HG13	1:C:546:PHE:HB2	1.96	0.47
1:A:81:TRP:HA	1:A:90:TYR:O	2.15	0.46
1:C:223:ARG:NH2	1:C:397:PRO:CG	2.79	0.46
1:C:541:VAL:CG1	1:C:546:PHE:HB2	2.45	0.46
1:A:52:LEU:O	1:A:107:LEU:HD11	2.15	0.46
1:B:130:VAL:HG22	1:B:173:ILE:HD11	1.98	0.46
1:D:152:ARG:NH1	1:D:162:GLU:OE2	2.48	0.46
1:D:289:ARG:HA	1:D:324:ALA:O	2.16	0.46
1:C:310:TYR:CE1	1:D:289:ARG:HD3	2.50	0.46
1:D:451:ARG:NH1	1:D:468:PRO:HG3	2.30	0.46
1:D:289:ARG:HG3	1:D:348:ILE:CD1	2.40	0.46
1:A:466:GLU:N	1:A:466:GLU:CD	2.68	0.46
1:C:42:ASN:HB2	4:C:5194:HOH:O	2.15	0.46
1:C:427:THR:OG1	1:C:428:PRO:HD3	2.15	0.46
1:C:187:ARG:HH11	1:C:187:ARG:HG3	1.81	0.46
1:C:409:ASN:N	1:C:409:ASN:ND2	2.63	0.46
1:C:35:HIS:HE1	1:C:175:GLU:HG2	1.81	0.46
1:A:201:ILE:HD11	1:A:366:LYS:HD3	1.97	0.46
1:C:253:LEU:HD21	1:C:437:ALA:HB1	1.98	0.46
1:D:96:ARG:HG3	1:D:400:THR:O	2.16	0.46
1:D:52:LEU:O	1:D:107:LEU:CD1	2.59	0.46
1:A:280:ASP:C	1:A:282:PRO:HD3	2.36	0.46
1:B:11:CYS:HA	1:B:28:GLY:O	2.17	0.46
1:B:47:PHE:CD2	1:B:48:MET:HE2	2.51	0.46
1:B:542:THR:OG1	1:B:545:ASN:HB2	2.16	0.46
1:C:403:VAL:HA	1:C:404:PRO:HD3	1.77	0.46
1:C:213:THR:HA	4:C:5224:HOH:O	2.15	0.45
1:C:219:ASP:O	1:C:223:ARG:HG3	2.16	0.45
1:A:86:LEU:HB2	1:A:89:THR:OG1	2.16	0.45
1:C:399:VAL:CG1	1:C:419:GLU:HB3	2.46	0.45
1:C:544:GLU:H	1:C:544:GLU:CD	2.19	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:557:LYS:HA	1:D:558:PRO:HD3	1.78	0.45
1:C:409:ASN:N	1:C:409:ASN:HD22	2.02	0.45
1:A:397:PRO:HG3	1:A:424:PRO:HG3	1.98	0.45
1:B:566:VAL:HG12	1:B:567:LEU:N	2.32	0.45
1:C:236:ARG:NH2	4:C:5056:HOH:O	2.49	0.45
1:A:420:GLU:OE1	1:A:420:GLU:HA	2.16	0.45
1:C:111:GLY:O	1:C:112:LYS:HB3	2.17	0.45
1:A:570:ASP:OD1	1:A:571:THR:N	2.48	0.45
1:B:267:GLU:HA	1:B:268:PRO:HD3	1.80	0.45
1:D:320:GLY:O	1:D:322:GLU:N	2.49	0.45
1:D:76:ARG:NH2	1:D:410:GLY:O	2.50	0.45
1:B:515:GLU:H	1:B:515:GLU:CD	2.20	0.45
1:D:48:MET:O	1:D:52:LEU:HG	2.17	0.45
1:A:222:VAL:HG12	1:A:427:THR:HG22	1.99	0.45
1:C:313:ASN:CG	4:C:5269:HOH:O	2.55	0.45
1:D:317:LYS:HE2	4:D:3371:HOH:O	2.17	0.45
1:D:407:LYS:HB2	1:D:409:ASN:HD21	1.82	0.45
1:A:536:LYS:HE2	1:A:554:MET:HE2	1.99	0.44
1:C:227:ARG:HG2	1:C:227:ARG:O	2.18	0.44
1:C:236:ARG:NH2	1:C:237:PHE:HZ	2.14	0.44
1:D:363:PHE:CE1	1:D:385:MET:CE	3.00	0.44
1:A:188:MET:HB3	4:A:729:HOH:O	2.17	0.44
1:C:423:ASP:HA	1:C:424:PRO:HD3	1.83	0.44
1:C:47:PHE:CD2	1:C:48:MET:HE2	2.52	0.44
1:A:82:SER:HB3	1:A:89:THR:HG21	1.93	0.44
1:C:203:THR:HG22	1:C:205:LYS:N	2.31	0.44
1:B:25:TRP:CD2	1:B:152:ARG:HD3	2.53	0.44
1:B:28:GLY:HA2	1:B:39:LYS:O	2.17	0.44
1:C:308:ARG:NH1	1:C:308:ARG:HG3	2.32	0.44
1:C:48:MET:CE	1:C:48:MET:HA	2.46	0.44
1:C:196:LYS:NZ	4:C:5219:HOH:O	2.50	0.44
1:D:400:THR:OG1	1:D:419:GLU:HA	2.17	0.44
1:B:157:LYS:HG3	1:B:157:LYS:O	2.18	0.44
1:D:68:ALA:CB	1:D:565:VAL:HG23	2.48	0.44
1:D:496:ARG:CG	1:D:496:ARG:NH1	2.81	0.44
1:D:553:LYS:HG2	1:D:571:THR:OG1	2.18	0.44
1:A:271:PHE:CZ	1:A:275:TYR:HB2	2.53	0.44
1:B:574:ILE:HA	4:B:743:HOH:O	2.16	0.44
1:C:353:PHE:CD1	1:C:353:PHE:N	2.86	0.44
1:A:206:LYS:O	1:A:210:VAL:HG23	2.17	0.44
1:C:503:ASP:HB3	1:C:524:ILE:CG2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:210:VAL:HG23	1:D:211:PHE:CD1	2.53	0.44
1:A:414:PHE:CD1	1:A:414:PHE:N	2.86	0.43
1:C:223:ARG:NH2	1:C:424:PRO:CG	2.60	0.43
1:C:319:SER:HB2	1:C:322:GLU:O	2.18	0.43
1:C:48:MET:CE	1:C:51:VAL:HG21	2.47	0.43
1:D:206:LYS:O	1:D:210:VAL:HG22	2.18	0.43
1:B:434:THR:HG22	1:B:438:ARG:NH1	2.33	0.43
1:B:552:ARG:HG2	1:B:554:MET:SD	2.58	0.43
1:C:267:GLU:HA	1:C:268:PRO:HD3	1.72	0.43
1:C:415:ARG:O	1:C:417:GLY:N	2.51	0.43
1:D:394:ALA:HB3	4:D:3238:HOH:O	2.17	0.43
1:A:86:LEU:H	1:A:89:THR:HB	1.83	0.43
1:C:289:ARG:CZ	1:C:348:ILE:HD11	2.48	0.43
1:C:536:LYS:HE2	1:C:554:MET:CE	2.48	0.43
1:D:495:LEU:HG	1:D:546:PHE:CE2	2.53	0.43
1:C:409:ASN:ND2	1:C:411:ALA:H	2.17	0.43
1:A:96:ARG:NH2	4:A:594:HOH:O	2.51	0.43
1:D:302:ILE:HD11	1:D:336:MET:CG	2.49	0.43
1:D:50:TRP:CE2	1:D:54:VAL:HG11	2.54	0.43
1:A:158:ILE:HG23	1:A:162:GLU:HB2	2.00	0.43
1:A:171:GLN:O	1:A:175:GLU:HG3	2.19	0.43
1:A:204:THR:CG2	1:A:208:LYS:HE3	2.49	0.43
1:C:223:ARG:NH1	1:C:223:ARG:HG2	2.33	0.43
1:C:67:GLY:O	1:C:71:ILE:HG12	2.18	0.43
1:A:89:THR:CG2	1:A:90:TYR:N	2.80	0.43
1:B:131:LYS:HG2	4:B:589:HOH:O	2.18	0.43
1:B:396:ASN:HA	1:B:397:PRO:HD3	1.89	0.43
1:C:118:VAL:HG11	1:C:120:TYR:CZ	2.53	0.43
1:C:249:ASP:HB2	1:C:486:GLU:CG	2.48	0.43
1:D:409:ASN:N	1:D:409:ASN:ND2	2.66	0.43
1:B:204:THR:O	1:B:208:LYS:HG3	2.18	0.43
1:D:133:ILE:O	1:D:137:PHE:HB2	2.19	0.43
1:B:557:LYS:HA	1:B:558:PRO:HD3	1.89	0.43
1:A:171:GLN:NE2	4:A:602:HOH:O	2.52	0.42
1:C:187:ARG:HD3	1:C:196:LYS:HD2	2.01	0.42
1:B:187:ARG:HB3	1:B:192:SER:CB	2.48	0.42
1:C:303:GLN:HG2	4:C:5337:HOH:O	2.18	0.42
1:C:50:TRP:CZ2	1:C:54:VAL:HG11	2.54	0.42
1:B:201:ILE:HD11	1:B:366:LYS:HD3	2.00	0.42
1:B:407:LYS:N	1:B:411:ALA:O	2.52	0.42
1:C:399:VAL:O	1:C:419:GLU:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:439:TYR:O	1:D:443:THR:HG23	2.20	0.42
1:C:476:ASP:HA	1:C:477:PRO:HD3	1.90	0.42
1:C:525:LYS:HD3	4:C:5314:HOH:O	2.19	0.42
1:D:292:PHE:CE2	1:D:319:SER:HB3	2.55	0.42
1:A:102:MET:HG2	1:A:103:ILE:N	2.30	0.42
1:A:496:ARG:HG3	1:A:496:ARG:NH1	2.32	0.42
1:B:281:TYR:N	1:B:282:PRO:HD3	2.34	0.42
1:B:476:ASP:HA	1:B:477:PRO:HD3	1.85	0.42
1:C:73:TRP:CZ3	1:C:74:LEU:HD23	2.54	0.42
1:C:75:GLU:HA	1:C:75:GLU:OE1	2.19	0.42
1:D:48:MET:HG3	1:D:73:TRP:CD2	2.55	0.42
1:A:210:VAL:C	1:A:212:PRO:HD3	2.40	0.42
1:A:31:ASN:HD22	1:A:33:GLU:H	1.67	0.42
1:A:395:SER:O	1:A:397:PRO:HD3	2.18	0.42
1:A:549:GLY:O	1:A:550:PHE:C	2.58	0.42
1:A:64:LYS:HG3	1:A:100:TRP:CD1	2.54	0.42
1:C:371:LYS:HD2	1:C:371:LYS:C	2.40	0.42
1:D:555:LYS:HD3	1:D:557:LYS:HE3	2.01	0.42
1:A:407:LYS:HE3	1:A:413:GLY:CA	2.49	0.42
1:B:217:GLY:O	1:B:221:GLU:HG3	2.20	0.42
1:A:323:ILE:CG1	1:B:307:SER:OG	2.67	0.42
1:D:409:ASN:ND2	1:D:411:ALA:H	2.17	0.42
1:A:328:LEU:HD12	1:A:333:LEU:HD13	2.02	0.42
1:A:493:LYS:HE2	1:A:495:LEU:HD21	2.01	0.42
1:A:50:TRP:CZ2	1:A:54:VAL:HG11	2.54	0.42
1:B:307:SER:HB2	1:B:308:ARG:H	1.57	0.42
1:B:545:ASN:ND2	1:B:550:PHE:CE1	2.86	0.42
1:B:554:MET:O	1:B:556:PRO:HD3	2.20	0.42
1:C:93:ILE:HD12	1:C:102:MET:HB3	2.02	0.42
1:A:80:LYS:HE2	4:A:592:HOH:O	2.19	0.42
1:C:268:PRO:HG3	1:C:353:PHE:CD2	2.55	0.42
1:D:25:TRP:CD2	1:D:152:ARG:HD3	2.55	0.42
1:B:507:LYS:HG3	1:B:509:VAL:HG23	2.01	0.41
1:C:187:ARG:HB3	1:C:192:SER:HB2	2.03	0.41
1:D:201:ILE:HD13	1:D:363:PHE:HA	2.02	0.41
1:D:23:ARG:HH22	1:D:153:PRO:HA	1.85	0.41
1:D:276:VAL:O	1:D:277:TRP:C	2.59	0.41
1:B:286:GLN:HG3	1:B:288:ILE:HG22	2.01	0.41
1:D:510:ASP:C	1:D:512:LYS:H	2.23	0.41
1:A:31:ASN:HB3	1:A:34:ASP:O	2.20	0.41
1:A:403:VAL:HA	1:A:404:PRO:HD3	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:495:LEU:HG	1:A:546:PHE:CE2	2.55	0.41
1:B:218:LEU:HD23	1:B:218:LEU:HA	1.87	0.41
1:D:284:HIS:CE1	1:D:330:ASN:HB3	2.55	0.41
1:A:227:ARG:HB2	1:A:438:ARG:NH1	2.35	0.41
1:A:550:PHE:HB3	1:A:574:ILE:HD12	2.03	0.41
1:B:276:VAL:O	1:B:277:TRP:C	2.58	0.41
1:B:11:CYS:SG	1:B:58:LEU:HB3	2.61	0.41
1:B:63:LEU:O	1:B:67:GLY:N	2.47	0.41
1:C:202:ILE:HG22	4:C:5286:HOH:O	2.21	0.41
1:A:61:HIS:O	1:A:62:ASN:CB	2.69	0.41
1:B:275:TYR:HE1	1:B:352:LYS:HG2	1.86	0.41
1:C:38:TYR:HE1	1:C:163:TYR:HH	1.67	0.41
1:C:405:TYR:HE2	1:C:415:ARG:HG3	1.86	0.41
1:D:363:PHE:CZ	1:D:385:MET:CE	2.98	0.41
1:A:496:ARG:CG	1:A:496:ARG:NH1	2.84	0.41
1:C:284:HIS:CE1	1:C:330:ASN:HB3	2.56	0.41
1:C:400:THR:CG2	1:C:416:LEU:HD22	2.51	0.41
1:C:86:LEU:O	1:C:87:PRO:C	2.58	0.41
1:D:61:HIS:O	1:D:62:ASN:CB	2.69	0.41
1:A:23:ARG:NH2	4:A:769:HOH:O	2.53	0.41
1:A:300:PRO:HB2	1:A:315:TYR:HB3	2.01	0.41
1:A:75:GLU:CB	1:A:406:LEU:HD11	2.33	0.41
1:B:275:TYR:CE1	1:B:352:LYS:HG2	2.55	0.41
1:B:48:MET:O	1:B:52:LEU:HG	2.20	0.41
1:D:102:MET:HG2	1:D:103:ILE:N	2.35	0.40
1:B:305:LYS:HE3	1:B:326:LEU:HD23	2.02	0.40
1:B:517:SER:HB2	1:B:518:PRO:CD	2.51	0.40
1:B:68:ALA:CB	1:B:565:VAL:HG23	2.51	0.40
1:C:506:MET:HB3	1:C:513:LEU:HG	2.03	0.40
1:D:191:GLY:O	1:D:392:LYS:HG3	2.21	0.40
1:D:409:ASN:HD22	1:D:410:GLY:N	2.19	0.40
1:B:561:VAL:HG13	1:B:562:PRO:CD	2.50	0.40
1:D:14:GLU:HB3	1:D:25:TRP:CE2	2.56	0.40
1:A:304:ILE:CD1	1:A:326:LEU:HD21	2.52	0.40
1:A:551:SER:HA	1:A:572:PHE:O	2.22	0.40
1:B:15:THR:HG21	1:B:69:PHE:CZ	2.56	0.40
1:B:27:TYR:CD2	1:B:47:PHE:HB2	2.56	0.40
1:B:31:ASN:HB3	1:B:34:ASP:O	2.21	0.40
1:B:73:TRP:CE3	1:B:74:LEU:HD23	2.57	0.40
1:C:25:TRP:CE3	1:C:26:ALA:HB2	2.56	0.40
1:D:236:ARG:NH1	4:D:3092:HOH:O	2.55	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	569/575 (99%)	518 (91%)	44 (8%)	7 (1%)	15	14
1	B	569/575 (99%)	521 (92%)	44 (8%)	4 (1%)	25	27
1	C	569/575 (99%)	525 (92%)	36 (6%)	8 (1%)	13	11
1	D	569/575 (99%)	536 (94%)	28 (5%)	5 (1%)	20	21
All	All	2276/2300 (99%)	2100 (92%)	152 (7%)	24 (1%)	17	16

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	62	ASN
1	A	311	LYS
1	B	311	LYS
1	D	62	ASN
1	A	85	GLY
1	A	310	TYR
1	C	416	LEU
1	D	312	GLY
1	D	321	GLY
1	A	309	PHE
1	B	127	PRO
1	C	187	ARG
1	C	426	TYR
1	C	203	THR
1	C	398	ASP
1	C	457	THR
1	D	320	GLY
1	D	457	THR
1	A	426	TYR
1	C	424	PRO

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Mol	Chain	Res	Type
1	B	457	THR
1	B	312	GLY
1	C	87	PRO
1	A	127	PRO

5.3.2 Protein sidechains ⓘ

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	502/506 (99%)	492 (98%)	10 (2%)	60	73
1	B	502/506 (99%)	493 (98%)	9 (2%)	64	76
1	C	502/506 (99%)	491 (98%)	11 (2%)	57	70
1	D	502/506 (99%)	496 (99%)	6 (1%)	75	86
All	All	2008/2024 (99%)	1972 (98%)	36 (2%)	64	76

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	GLU
1	A	31	ASN
1	A	145	ASP
1	A	185	LEU
1	A	249	ASP
1	A	318	SER
1	A	390	TYR
1	A	396	ASN
1	A	414	PHE
1	A	466	GLU
1	B	16	THR
1	B	31	ASN
1	B	88	ASN
1	B	116	HIS
1	B	128	PHE
1	B	145	ASP
1	B	223	ARG

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Mol	Chain	Res	Type
1	B	249	ASP
1	B	552	ARG
1	C	89	THR
1	C	145	ASP
1	C	186	ASP
1	C	187	ARG
1	C	219	ASP
1	C	249	ASP
1	C	304	ILE
1	C	314	GLU
1	C	390	TYR
1	C	409	ASN
1	C	420	GLU
1	D	31	ASN
1	D	54	VAL
1	D	310	TYR
1	D	311	LYS
1	D	384	LEU
1	D	409	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	35	HIS
1	A	72	ASN
1	A	171	GLN
1	A	287	HIS
1	A	380	GLN
1	A	396	ASN
1	B	31	ASN
1	B	116	HIS
1	B	171	GLN
1	B	287	HIS
1	B	313	ASN
1	B	396	ASN
1	B	545	ASN
1	C	31	ASN
1	C	35	HIS
1	C	55	GLN
1	C	171	GLN
1	C	313	ASN

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Mol	Chain	Res	Type
1	C	409	ASN
1	C	545	ASN
1	D	31	ASN
1	D	35	HIS
1	D	171	GLN
1	D	287	HIS
1	D	303	GLN
1	D	409	ASN
1	D	485	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	SO4	D	3000	-	4,4,4	1.81	1 (25%)	6,6,6	0.92	0
2	SO4	D	3001	-	4,4,4	1.92	1 (25%)	6,6,6	0.83	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	SO4	D	3000	-	-	0/0/0/0	0/0/0/0
2	SO4	D	3001	-	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	3000	SO4	O1-S	2.99	1.61	1.45
2	D	3001	SO4	O1-S	3.36	1.63	1.45

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](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	571/575 (99%)	0.71	83 (14%) 3 5	25, 55, 108, 135	0
1	B	571/575 (99%)	0.58	63 (11%) 6 10	23, 50, 95, 149	0
1	C	571/575 (99%)	0.55	62 (10%) 6 10	22, 47, 106, 147	0
1	D	571/575 (99%)	0.28	28 (4%) 30 42	22, 43, 84, 150	0
All	All	2284/2300 (99%)	0.53	236 (10%) 7 11	22, 48, 103, 150	0

All (236) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	310	TYR	11.3
1	D	306	ARG	8.7
1	A	148	TYR	8.5
1	B	310	TYR	8.3
1	A	309	PHE	8.1
1	C	400	THR	8.0
1	C	421	THR	8.0
1	A	306	ARG	7.7
1	A	399	VAL	7.3
1	B	113	ARG	7.2
1	B	311	LYS	7.1
1	A	310	TYR	7.0
1	D	308	ARG	6.7
1	B	149	HIS	6.4
1	A	307	SER	6.4
1	A	405	TYR	6.2
1	A	512	LYS	6.0
1	A	308	ARG	6.0
1	C	420	GLU	5.9
1	B	309	PHE	5.6
1	B	109	TYR	5.6

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Mol	Chain	Res	Type	RSRZ
1	C	423	ASP	5.5
1	A	5	PRO	5.5
1	C	5	PRO	5.2
1	C	115	ILE	5.2
1	C	309	PHE	5.1
1	C	419	GLU	5.0
1	B	86	LEU	5.0
1	A	311	LYS	4.9
1	A	312	GLY	4.8
1	A	149	HIS	4.8
1	A	510	ASP	4.8
1	C	418	GLU	4.7
1	D	307	SER	4.6
1	C	310	TYR	4.6
1	A	509	VAL	4.5
1	C	111	GLY	4.5
1	B	5	PRO	4.5
1	A	111	GLY	4.4
1	C	113	ARG	4.4
1	A	416	LEU	4.3
1	A	559	VAL	4.3
1	D	148	TYR	4.3
1	A	151	GLU	4.3
1	C	149	HIS	4.3
1	A	575	LYS	4.1
1	A	419	GLU	4.0
1	C	108	GLY	4.0
1	B	575	LYS	4.0
1	C	53	LYS	4.0
1	C	112	LYS	3.9
1	A	216	LEU	3.9
1	C	398	ASP	3.9
1	A	572	PHE	3.9
1	C	575	LYS	3.8
1	B	510	ASP	3.8
1	B	312	GLY	3.8
1	C	304	ILE	3.8
1	A	422	LYS	3.7
1	D	149	HIS	3.7
1	A	403	VAL	3.7
1	C	422	LYS	3.6
1	A	313	ASN	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	309	PHE	3.6
1	B	11	CYS	3.5
1	C	553	LYS	3.5
1	A	564	GLY	3.5
1	B	108	GLY	3.5
1	C	148	TYR	3.5
1	A	153	PRO	3.4
1	C	116	HIS	3.4
1	A	508	GLU	3.4
1	A	11	CYS	3.4
1	B	111	GLY	3.3
1	D	511	GLY	3.3
1	D	570	ASP	3.3
1	C	85	GLY	3.3
1	A	112	LYS	3.3
1	C	107	LEU	3.3
1	A	415	ARG	3.3
1	D	508	GLU	3.3
1	B	151	GLU	3.3
1	D	311	LYS	3.2
1	C	110	LYS	3.2
1	D	512	LYS	3.2
1	B	419	GLU	3.2
1	C	572	PHE	3.2
1	C	311	LYS	3.2
1	A	97	MET	3.1
1	A	409	ASN	3.1
1	A	85	GLY	3.1
1	C	571	THR	3.1
1	C	119	ILE	3.1
1	C	399	VAL	3.1
1	B	304	ILE	3.1
1	B	154	VAL	3.0
1	B	85	GLY	3.0
1	B	97	MET	3.0
1	B	421	THR	2.9
1	C	11	CYS	2.9
1	B	28	GLY	2.9
1	B	70	ILE	2.9
1	A	328	LEU	2.9
1	B	96	ARG	2.9
1	C	84	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	308	ARG	2.8
1	A	154	VAL	2.8
1	C	12	ALA	2.8
1	A	75	GLU	2.8
1	A	305	LYS	2.8
1	B	157	LYS	2.8
1	B	400	THR	2.8
1	D	575	LYS	2.8
1	C	397	PRO	2.7
1	B	53	LYS	2.7
1	D	523	ASP	2.7
1	B	148	TYR	2.7
1	B	435	ALA	2.7
1	A	395	SER	2.7
1	B	12	ALA	2.7
1	B	66	ALA	2.7
1	A	157	LYS	2.7
1	A	410	GLY	2.7
1	B	569	ASP	2.6
1	D	431	VAL	2.6
1	B	433	ILE	2.6
1	A	431	VAL	2.6
1	B	418	GLU	2.6
1	A	70	ILE	2.6
1	B	532	GLY	2.6
1	C	67	GLY	2.6
1	A	400	THR	2.6
1	C	509	VAL	2.6
1	C	13	PHE	2.6
1	A	511	GLY	2.6
1	A	404	PRO	2.5
1	A	513	LEU	2.5
1	A	60	PHE	2.5
1	C	331	VAL	2.5
1	B	165	TYR	2.5
1	C	225	ALA	2.5
1	A	96	ARG	2.5
1	A	418	GLU	2.5
1	B	106	CYS	2.5
1	D	408	GLU	2.5
1	C	181	PHE	2.5
1	D	510	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	313	ASN	2.5
1	A	544	GLU	2.4
1	A	413	GLY	2.4
1	C	186	ASP	2.4
1	C	415	ARG	2.4
1	A	20	GLU	2.4
1	A	397	PRO	2.4
1	B	105	ILE	2.4
1	C	424	PRO	2.4
1	A	423	ASP	2.4
1	D	522	THR	2.4
1	C	59	TYR	2.4
1	A	227	ARG	2.4
1	B	399	VAL	2.4
1	C	511	GLY	2.4
1	B	117	THR	2.4
1	C	184	GLY	2.3
1	A	421	THR	2.3
1	A	434	THR	2.3
1	B	118	VAL	2.3
1	C	512	LYS	2.3
1	A	570	ASP	2.3
1	B	67	GLY	2.3
1	C	66	ALA	2.3
1	D	435	ALA	2.3
1	A	565	VAL	2.3
1	B	572	PHE	2.3
1	C	114	LYS	2.3
1	A	573	THR	2.3
1	B	156	TYR	2.3
1	D	328	LEU	2.3
1	C	10	SER	2.3
1	D	333	LEU	2.3
1	B	119	ILE	2.3
1	A	407	LYS	2.2
1	B	512	LYS	2.2
1	D	112	LYS	2.2
1	C	510	ASP	2.2
1	D	520	ASP	2.2
1	B	398	ASP	2.2
1	C	60	PHE	2.2
1	A	83	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	328	LEU	2.2
1	D	513	LEU	2.2
1	C	109	TYR	2.2
1	A	373	THR	2.2
1	B	80	LYS	2.2
1	A	65	PHE	2.2
1	A	435	ALA	2.2
1	B	305	LYS	2.2
1	C	58	LEU	2.2
1	A	186	ASP	2.2
1	B	554	MET	2.2
1	B	307	SER	2.2
1	A	155	GLY	2.2
1	C	308	ARG	2.1
1	A	571	THR	2.1
1	B	571	THR	2.1
1	A	420	GLU	2.1
1	A	402	LYS	2.1
1	A	560	GLN	2.1
1	A	398	ASP	2.1
1	C	305	LYS	2.1
1	D	331	VAL	2.1
1	A	414	PHE	2.1
1	B	13	PHE	2.1
1	B	44	LEU	2.1
1	C	63	LEU	2.1
1	B	107	LEU	2.1
1	A	113	ARG	2.1
1	C	431	VAL	2.1
1	D	312	GLY	2.1
1	C	70	ILE	2.1
1	B	570	ASP	2.0
1	B	41	GLY	2.0
1	B	153	PRO	2.0
1	B	422	LYS	2.0
1	A	119	ILE	2.0
1	A	396	ASN	2.0
1	A	532	GLY	2.0
1	A	147	ASP	2.0
1	B	423	ASP	2.0
1	C	570	ASP	2.0
1	A	539	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	110	LYS	2.0
1	D	399	VAL	2.0
1	A	12	ALA	2.0
1	A	411	ALA	2.0
1	B	553	LYS	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	MG	C	5000	1/1	0.95	0.22	2.66	47,47,47,47	0
3	MG	C	5001	1/1	0.88	0.18	0.21	53,53,53,53	0
2	SO4	D	3000	5/5	0.97	0.16	-	67,75,77,83	0
2	SO4	D	3001	5/5	0.93	0.19	-	98,99,102,103	0

6.5 Other polymers [i](#)

There are no such residues in this entry.