Full wwPDB X-ray Structure Validation Report ⓘ

Oct 12, 2021 – 03:17 PM EDT

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
https://www.wwpdb.org/validation/2017/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:

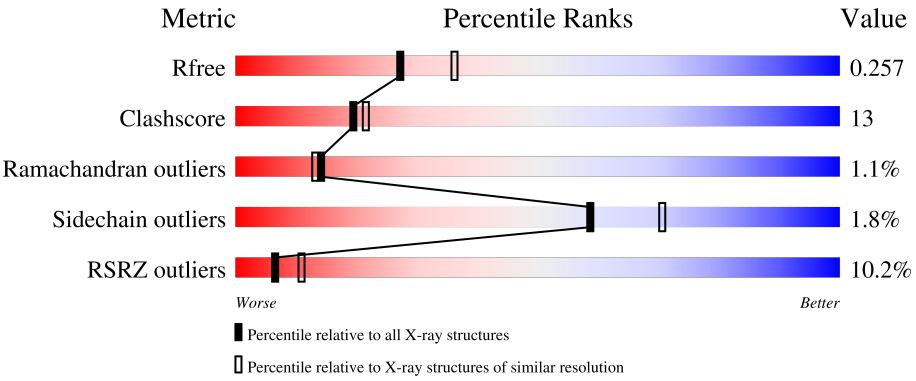
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 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}	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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	575	14% 73% 25%
1	B	575	11% 72% 26%
1	C	575	11% 73% 25%
1	D	575	5% 79% 19%

2 Entry composition (i)

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			

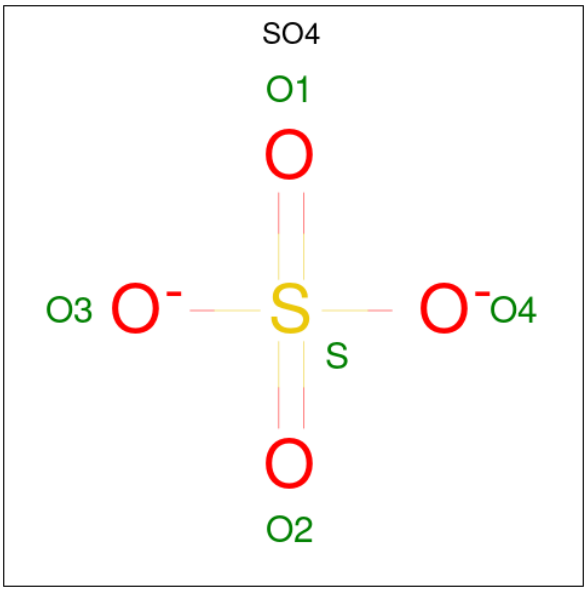
There are 8 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 4 is water.

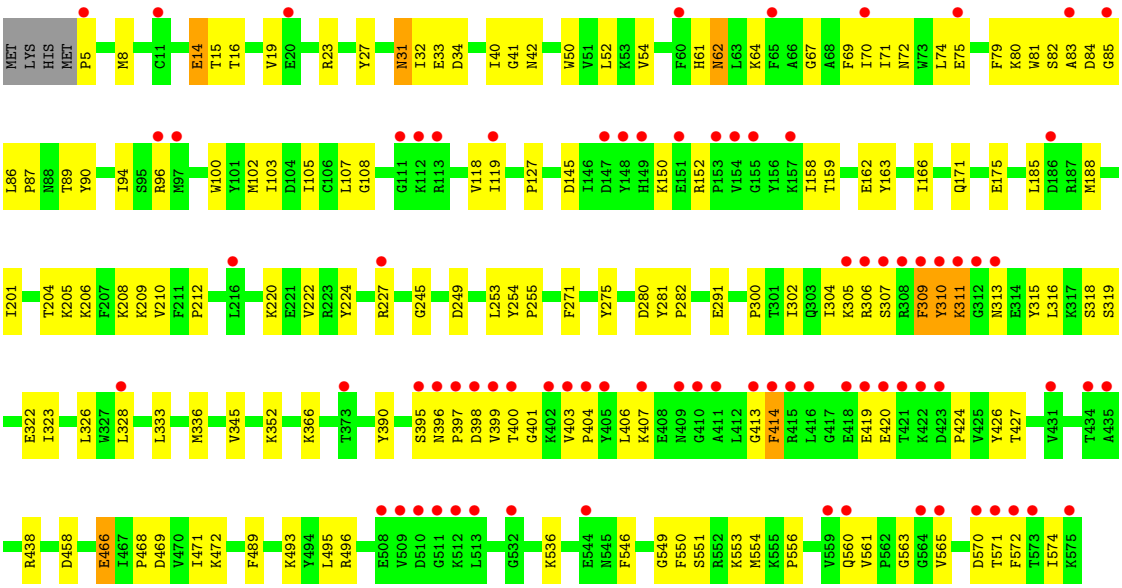
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	295	Total O 295 295	0	0
4	B	388	Total O 388 388	0	0
4	C	382	Total O 382 382	0	0
4	D	444	Total O 444 444	0	0

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.

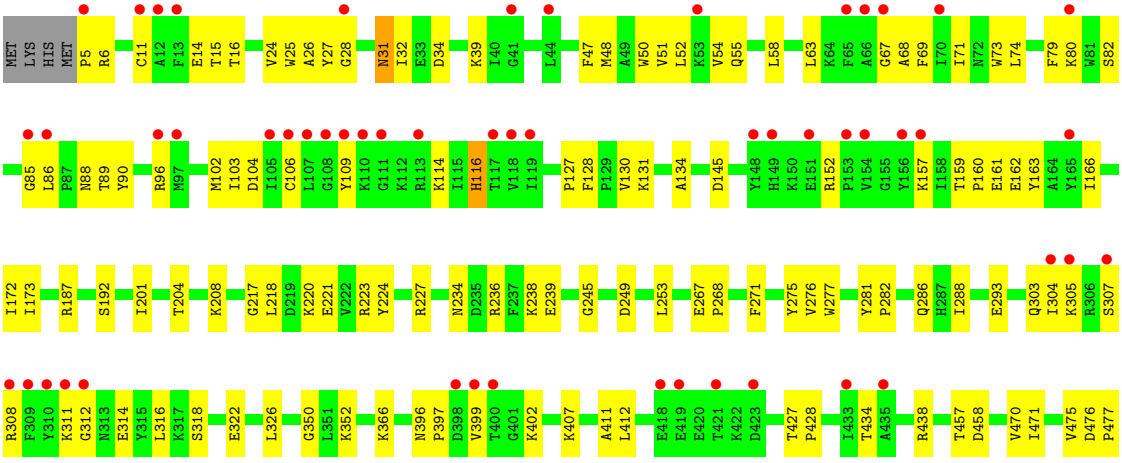
• Molecule 1: DNA polymerase

Chain A:



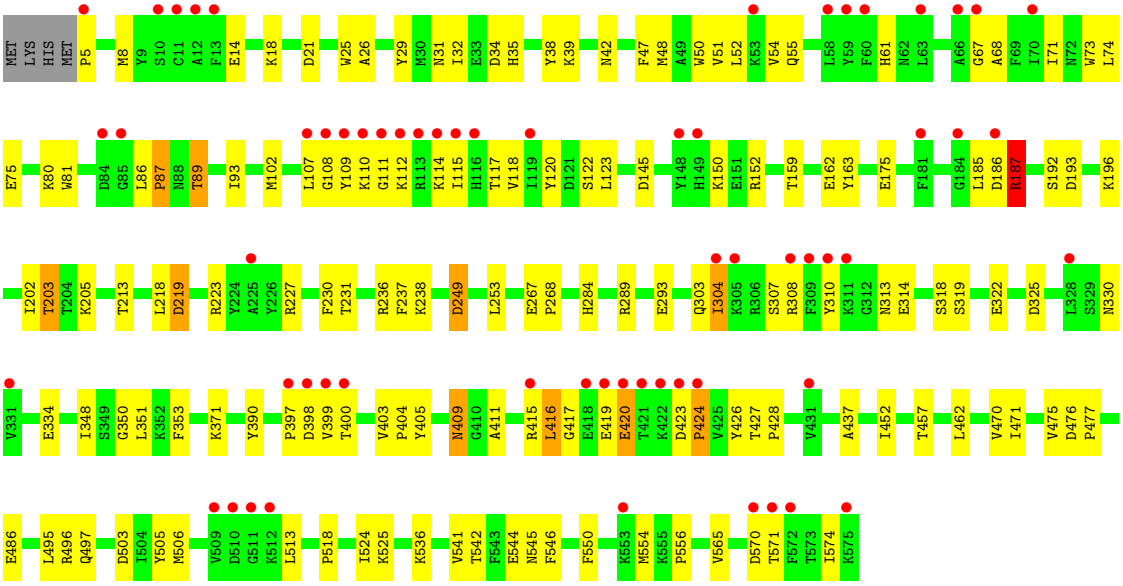
• Molecule 1: DNA polymerase

Chain B:



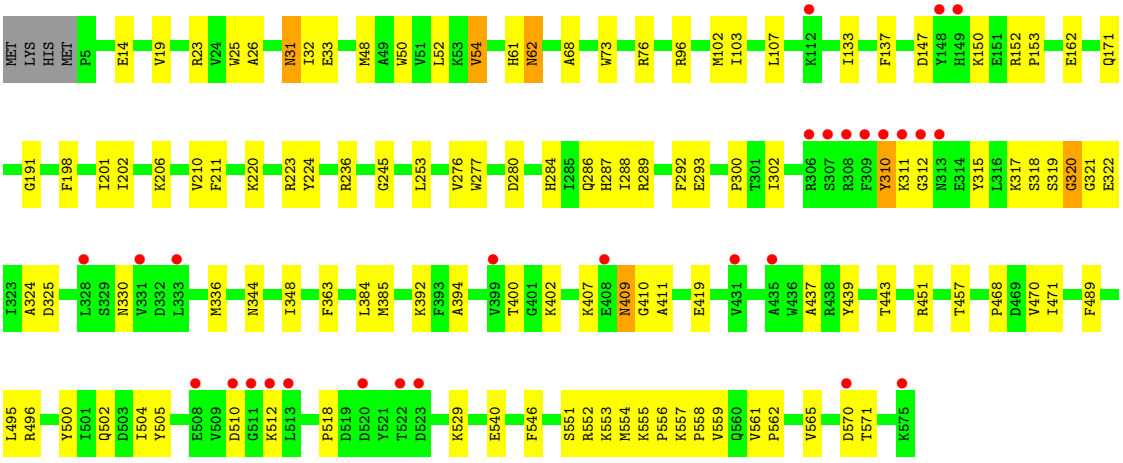
• Molecule 1: DNA polymerase

Chain C:



• Molecule 1: DNA polymerase

Chain D:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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	12006 reflections (10.01%)	wwPDB-VP
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]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	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.*

[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: SO4, MG

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(^{o})	Ideal(^{o})
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	C	2	0	0	0	0
3	D	10	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:82:SER:HB3	1:A:89:THR:CG2	2.10	0.81
1:A:310:TYR:HH	1:A:322:GLU:HG3	1.43	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:HH11	1:D:496:ARG:HG3	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:302:ILE:HD11	1:D:336:MET:SD	2.36	0.65
1:D:310:TYR:N	1:D:310:TYR:CD2	2.61	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:B:5:PRO:CG	1:C:5:PRO:HG3	2.31	0.61
1:C:61:HIS:O	1:C:123:LEU:HB2	2.01	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:HG12	1:B:399:VAL:O	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:C	1:A:31:ASN:HD22	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:CD	1:A:466:GLU:H	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:HD2	1:C:187:ARG:N	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:HD22	1:D:31:ASN:C	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:OE1	1:A:14:GLU:HA	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:253:LEU:HD22	1:B:458:ASP:HB3	1.89	0.53
1:B:427:THR:OG1	1:B:428:PRO:HD3	2.09	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:75:GLU:CG	1:A:406:LEU:HD21	2.38	0.53
1:A:302:ILE:HD11	1:A:336:MET:HG3	1.90	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:81:TRP:CD1	1:C:404:PRO:HD2	2.44	0.53
1:C:496:ARG:HG2	1:C:496:ARG:NH1	2.24	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:H	1:A:69:PHE:HD1	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:H	1:C:409:ASN:ND2	2.07	0.51
1:A:84:ASP:HB2	4:A:593:HOH:O	2.11	0.51
1:A:468:PRO:HD2	1:A:471:ILE:HD11	1.93	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:6:ARG:NH1	1:B:116:HIS:HE1	2.09	0.50
1:B:304:ILE:HD12	1:B:314:GLU:CD	2.32	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:19:VAL:HG13	1:A:561:VAL:HG11	1.94	0.50
1:A:40:ILE:HD12	1:A:163:TYR:CE1	2.47	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:86:LEU:O	1:B:89:THR:HB	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:495:LEU:HG	1:B:546:PHE:CE2	2.47	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:OD1	1:A:398:ASP:O	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:15:THR:HG21	1:A:69:PHE:CZ	2.49	0.48
1:A:100:TRP:N	1:A:100:TRP:CD1	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:B:227:ARG:HG2	1:B:227:ARG:HH11	1.79	0.47
1:A:102:MET:HG3	1:A:118:VAL:CG1	2.44	0.47
1:B:5:PRO:HG3	1:C:5:PRO:CB	2.44	0.47
1:B:160:PRO:O	1:B:163:TYR:HB3	2.14	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: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:D:31:ASN:HD22	1:D:32:ILE:N	2.13	0.47
1:C:308:ARG:HG3	1:C:308:ARG:HH11	1.80	0.47
1:A:319:SER:HB2	1:A:322:GLU:O	2.14	0.47
1:B:74:LEU:O	1:B:79:PHE:HB2	2.15	0.47
1:B:304:ILE:HG12	1:B:316:LEU:HD11	1.97	0.47
1:C:350:GLY:O	1:C:351:LEU:HD23	2.14	0.47
1:B:31:ASN:HD22	1:B:31:ASN:C	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:C:310:TYR:CE1	1:D:289:ARG:HD3	2.50	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: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:CD	1:A:466:GLU:N	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:HG3	1:C:187:ARG:HH11	1.81	0.46
1:C:409:ASN:ND2	1:C:409:ASN:N	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:52:LEU:O	1:D:107:LEU:CD1	2.59	0.46
1:D:96:ARG:HG3	1:D:400:THR:O	2.16	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:CD	1:C:544:GLU:H	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:HD22	1:C:409:ASN:N	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:76:ARG:NH2	1:D:410:GLY:O	2.50	0.45
1:D:320:GLY:O	1:D:322:GLU:N	2.49	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:O	1:C:227:ARG:HG2	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:47:PHE:CD2	1:C:48:MET:HE2	2.52	0.44
1:C:423:ASP:HA	1:C:424:PRO:HD3	1.83	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:48:MET:HA	1:C:48:MET:CE	2.46	0.44
1:C:308:ARG:HG3	1:C:308:ARG:NH1	2.32	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:O	1:B:157:LYS:HG3	2.18	0.44
1:D:68:ALA:CB	1:D:565:VAL:HG23	2.48	0.44
1:D:496:ARG:NH1	1:D:496:ARG:CG	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:N	1:A:414:PHE:CD1	2.86	0.43
1:C:48:MET:CE	1:C:51:VAL:HG21	2.47	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: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:50:TRP:CE2	1:D:54:VAL:HG11	2.54	0.43
1:D:302:ILE:HD11	1:D:336:MET:CG	2.49	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:67:GLY:O	1:C:71:ILE:HG12	2.18	0.43
1:C:223:ARG:HG2	1:C:223:ARG:NH1	2.33	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:50:TRP:CZ2	1:C:54:VAL:HG11	2.54	0.42
1:C:303:GLN:HG2	4:C:5337:HOH:O	2.18	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:OE1	1:C:75:GLU:HA	2.19	0.42
1:D:48:MET:HG3	1:D:73:TRP:CD2	2.55	0.42
1:A:31:ASN:HD22	1:A:33:GLU:H	1.67	0.42
1:A:64:LYS:HG3	1:A:100:TRP:CD1	2.54	0.42
1:A:210:VAL:C	1:A:212:PRO:HD3	2.40	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:C:371:LYS:C	1:C:371:LYS:HD2	2.40	0.42
1:D:555:LYS:HD3	1:D:557:LYS:HE3	2.01	0.42
1:A:323:ILE:CG1	1:B:307:SER:OG	2.67	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:D:409:ASN:ND2	1:D:411:ALA:H	2.17	0.42
1:A:50:TRP:CZ2	1:A:54:VAL:HG11	2.54	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: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:23:ARG:HH22	1:D:153:PRO:HA	1.85	0.41
1:D:201:ILE:HD13	1:D:363:PHE:HA	2.02	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: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:B:276:VAL:O	1:B:277:TRP:C	2.58	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:23:ARG:NH2	4:A:769:HOH:O	2.53	0.41
1:A:75:GLU:CB	1:A:406:LEU:HD11	2.33	0.41
1:A:300:PRO:HB2	1:A:315:TYR:HB3	2.01	0.41
1:A:496:ARG:NH1	1:A:496:ARG:CG	2.84	0.41
1:B:275:TYR:CE1	1:B:352:LYS:HG2	2.55	0.41
1:C:86:LEU:O	1:C:87:PRO:C	2.58	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:D:61:HIS:O	1:D:62:ASN:CB	2.69	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:68:ALA:CB	1:B:565:VAL:HG23	2.51	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: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%)	13 11
1	B	569/575 (99%)	521 (92%)	44 (8%)	4 (1%)	22 23
1	C	569/575 (99%)	525 (92%)	36 (6%)	8 (1%)	11 9
1	D	569/575 (99%)	536 (94%)	28 (5%)	5 (1%)	17 17
All	All	2276/2300 (99%)	2100 (92%)	152 (7%)	24 (1%)	14 13

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 (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	502/506 (99%)	492 (98%)	10 (2%)	55	66
1	B	502/506 (99%)	493 (98%)	9 (2%)	59	70
1	C	502/506 (99%)	491 (98%)	11 (2%)	52	63
1	D	502/506 (99%)	496 (99%)	6 (1%)	71	82
All	All	2008/2024 (99%)	1972 (98%)	36 (2%)	59	70

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

Sometimes 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 monosaccharides 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	$\#\|Z\| > 2$
3	SO4	D	3001	-	4,4,4	1.92	1 (25%)	6,6,6	0.86	0
3	SO4	D	3000	-	4,4,4	1.84	2 (50%)	6,6,6	0.95	0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	3001	SO4	O1-S	3.29	1.63	1.46
3	D	3000	SO4	O1-S	2.92	1.61	1.46
3	D	3000	SO4	O3-S	-2.12	1.30	1.47

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

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	571/575 (99%)	0.71	81 (14%) 2 4	25, 55, 108, 135	0
1	B	571/575 (99%)	0.58	62 (10%) 5 9	23, 50, 95, 149	0
1	C	571/575 (99%)	0.55	62 (10%) 5 9	22, 47, 106, 147	0
1	D	571/575 (99%)	0.27	28 (4%) 29 42	22, 43, 84, 150	0
All	All	2284/2300 (99%)	0.53	233 (10%) 6 11	22, 48, 103, 150	0

All (233) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	310	TYR	11.5
1	D	306	ARG	8.7
1	A	148	TYR	8.5
1	B	310	TYR	8.4
1	A	309	PHE	8.1
1	C	421	THR	8.0
1	C	400	THR	7.9
1	A	306	ARG	7.6
1	A	399	VAL	7.3
1	B	113	ARG	7.2
1	A	310	TYR	7.1
1	B	311	LYS	7.0
1	D	308	ARG	6.7
1	A	307	SER	6.4
1	B	149	HIS	6.3
1	A	405	TYR	6.2
1	A	512	LYS	6.0
1	A	308	ARG	6.0
1	C	420	GLU	5.8
1	B	309	PHE	5.7
1	C	423	ASP	5.6

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Mol	Chain	Res	Type	RSRZ
1	B	109	TYR	5.5
1	A	5	PRO	5.4
1	C	115	ILE	5.2
1	C	5	PRO	5.2
1	C	309	PHE	5.1
1	C	419	GLU	5.1
1	B	86	LEU	5.0
1	A	311	LYS	4.9
1	A	149	HIS	4.8
1	A	510	ASP	4.8
1	A	312	GLY	4.8
1	C	418	GLU	4.7
1	D	307	SER	4.6
1	A	509	VAL	4.6
1	C	310	TYR	4.5
1	B	5	PRO	4.5
1	C	111	GLY	4.4
1	C	113	ARG	4.4
1	A	416	LEU	4.4
1	A	111	GLY	4.4
1	D	148	TYR	4.3
1	A	151	GLU	4.3
1	A	559	VAL	4.3
1	C	149	HIS	4.3
1	A	575	LYS	4.1
1	A	419	GLU	4.1
1	C	53	LYS	4.0
1	C	112	LYS	4.0
1	C	108	GLY	4.0
1	A	216	LEU	4.0
1	B	575	LYS	3.9
1	B	312	GLY	3.8
1	A	572	PHE	3.8
1	C	398	ASP	3.8
1	C	575	LYS	3.8
1	B	510	ASP	3.8
1	C	304	ILE	3.7
1	D	149	HIS	3.7
1	A	422	LYS	3.7
1	A	403	VAL	3.7
1	C	422	LYS	3.7
1	A	313	ASN	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	309	PHE	3.6
1	C	553	LYS	3.6
1	A	564	GLY	3.4
1	C	148	TYR	3.4
1	B	11	CYS	3.4
1	B	108	GLY	3.4
1	A	508	GLU	3.4
1	A	11	CYS	3.4
1	C	116	HIS	3.4
1	A	153	PRO	3.4
1	D	511	GLY	3.3
1	D	570	ASP	3.3
1	B	111	GLY	3.3
1	A	112	LYS	3.3
1	D	508	GLU	3.3
1	C	107	LEU	3.3
1	A	415	ARG	3.3
1	D	311	LYS	3.2
1	C	110	LYS	3.2
1	C	85	GLY	3.2
1	B	151	GLU	3.2
1	C	572	PHE	3.2
1	A	97	MET	3.2
1	C	311	LYS	3.2
1	B	419	GLU	3.1
1	D	512	LYS	3.1
1	A	409	ASN	3.1
1	C	399	VAL	3.1
1	A	85	GLY	3.1
1	B	154	VAL	3.1
1	C	119	ILE	3.1
1	C	571	THR	3.1
1	B	85	GLY	3.1
1	B	304	ILE	3.0
1	B	97	MET	3.0
1	C	11	CYS	2.9
1	B	421	THR	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	C	397	PRO	2.7
1	B	400	THR	2.7
1	D	523	ASP	2.7
1	B	435	ALA	2.7
1	B	157	LYS	2.7
1	D	575	LYS	2.7
1	B	569	ASP	2.7
1	B	53	LYS	2.7
1	B	12	ALA	2.7
1	B	66	ALA	2.7
1	B	148	TYR	2.7
1	A	410	GLY	2.7
1	A	395	SER	2.6
1	A	157	LYS	2.6
1	B	433	ILE	2.6
1	B	532	GLY	2.6
1	C	509	VAL	2.6
1	B	418	GLU	2.6
1	A	400	THR	2.6
1	A	431	VAL	2.6
1	D	431	VAL	2.6
1	C	67	GLY	2.6
1	C	13	PHE	2.6
1	A	511	GLY	2.6
1	A	513	LEU	2.5
1	C	225	ALA	2.5
1	A	70	ILE	2.5
1	A	404	PRO	2.5
1	B	165	TYR	2.5
1	A	60	PHE	2.5
1	C	331	VAL	2.5
1	A	96	ARG	2.5
1	D	408	GLU	2.5
1	D	510	ASP	2.5
1	A	397	PRO	2.5
1	A	413	GLY	2.5
1	B	106	CYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	313	ASN	2.5
1	C	181	PHE	2.4
1	C	186	ASP	2.4
1	C	415	ARG	2.4
1	A	418	GLU	2.4
1	A	423	ASP	2.4
1	C	184	GLY	2.4
1	C	511	GLY	2.4
1	D	522	THR	2.4
1	A	227	ARG	2.4
1	A	544	GLU	2.4
1	B	105	ILE	2.4
1	A	20	GLU	2.4
1	C	424	PRO	2.4
1	C	59	TYR	2.4
1	B	118	VAL	2.4
1	B	399	VAL	2.4
1	B	117	THR	2.4
1	C	512	LYS	2.3
1	A	434	THR	2.3
1	A	565	VAL	2.3
1	D	435	ALA	2.3
1	A	421	THR	2.3
1	B	67	GLY	2.3
1	B	156	TYR	2.3
1	B	572	PHE	2.3
1	C	114	LYS	2.3
1	A	570	ASP	2.3
1	A	573	THR	2.3
1	C	10	SER	2.3
1	B	119	ILE	2.3
1	C	66	ALA	2.3
1	D	328	LEU	2.3
1	D	333	LEU	2.3
1	D	520	ASP	2.2
1	A	407	LYS	2.2
1	D	112	LYS	2.2
1	B	398	ASP	2.2
1	C	109	TYR	2.2
1	C	510	ASP	2.2
1	C	60	PHE	2.2
1	B	512	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	571	THR	2.2
1	C	328	LEU	2.2
1	B	305	LYS	2.2
1	B	307	SER	2.2
1	A	65	PHE	2.2
1	D	513	LEU	2.2
1	A	186	ASP	2.2
1	A	560	GLN	2.2
1	A	83	ALA	2.2
1	A	435	ALA	2.2
1	C	308	ARG	2.2
1	C	58	LEU	2.2
1	B	554	MET	2.2
1	A	398	ASP	2.2
1	B	80	LYS	2.1
1	A	373	THR	2.1
1	A	420	GLU	2.1
1	C	63	LEU	2.1
1	A	402	LYS	2.1
1	A	571	THR	2.1
1	A	113	ARG	2.1
1	C	305	LYS	2.1
1	D	331	VAL	2.1
1	B	13	PHE	2.1
1	A	155	GLY	2.1
1	B	110	LYS	2.1
1	B	107	LEU	2.1
1	A	411	ALA	2.1
1	C	431	VAL	2.1
1	A	414	PHE	2.1
1	A	119	ILE	2.1
1	B	44	LEU	2.1
1	C	70	ILE	2.1
1	B	570	ASP	2.1
1	B	423	ASP	2.0
1	B	41	GLY	2.0
1	B	153	PRO	2.0
1	A	147	ASP	2.0
1	D	399	VAL	2.0
1	B	65	PHE	2.0
1	A	532	GLY	2.0
1	D	312	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	396	ASN	2.0
1	C	570	ASP	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 monosaccharides 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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MG	C	5001	1/1	0.88	0.19	53,53,53,53	0
3	SO4	D	3001	5/5	0.93	0.19	98,99,102,103	0
2	MG	C	5000	1/1	0.95	0.22	47,47,47,47	0
3	SO4	D	3000	5/5	0.97	0.16	67,75,77,83	0

6.5 Other polymers (i)

There are no such residues in this entry.