



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 11:46 PM UTC

PDB ID : 1XHX / pdb_00001xhx
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 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

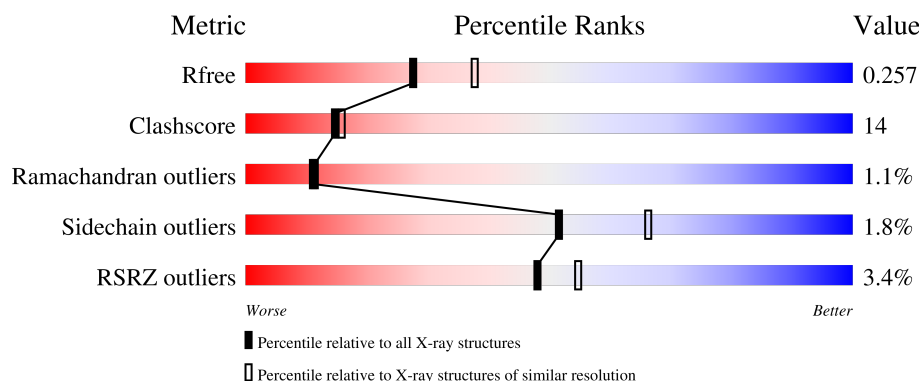
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (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 $\leq 5\%$. 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	6% 70% 27% ..
1	B	575	4% 69% 28% ..
1	C	575	3% 69% 28% ..
1	D	575	% 76% 22% ..

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			

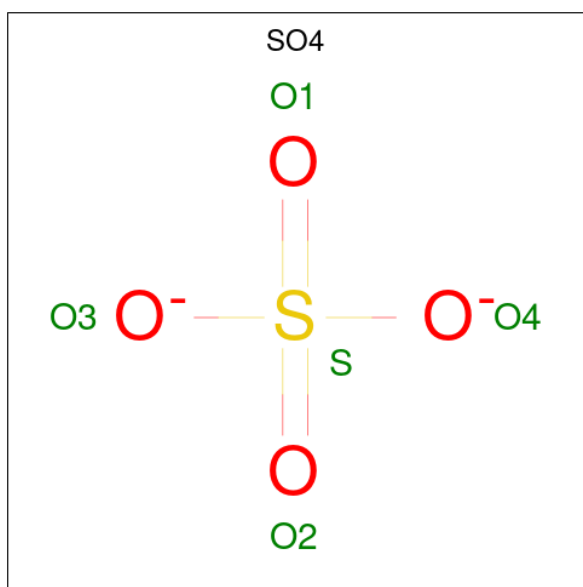
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	ALA	ASP	engineered 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 (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- 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		

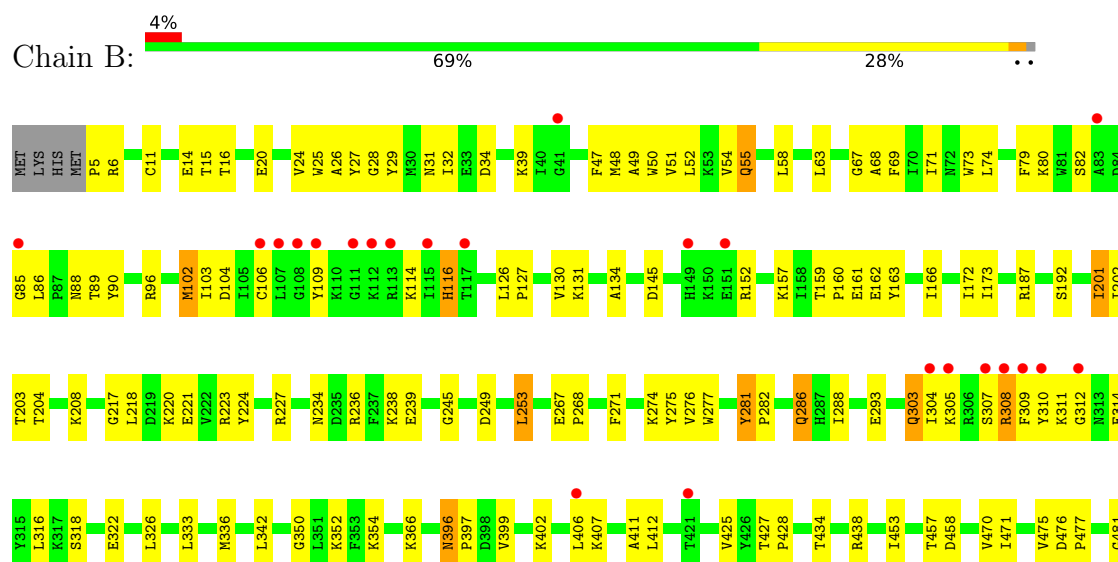
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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



• Molecule 1: DNA polymerase

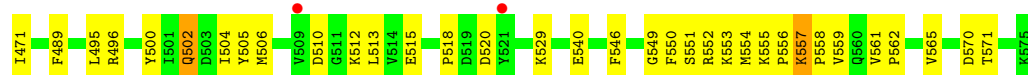
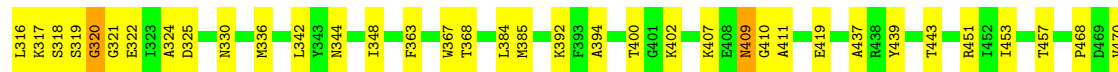
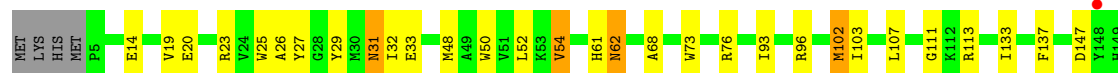
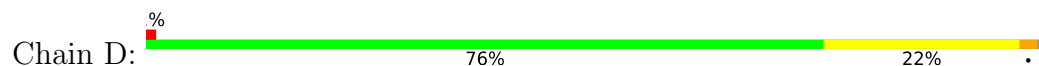




• Molecule 1: DNA polymerase



• 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 19.96 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.7 (19.96-2.35) 99.7 (19.96-2.35)	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	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)	0.33 , 48.1	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: 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	0.40	0/4788	0.99	24/6459 (0.4%)
1	B	0.41	0/4788	0.97	24/6459 (0.4%)
1	C	0.40	0/4788	0.95	29/6459 (0.4%)
1	D	0.43	0/4788	0.91	12/6459 (0.2%)
All	All	0.41	0/19152	0.95	89/25836 (0.3%)

There are no bond length outliers.

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	309	PHE	CA-CB-CG	-16.59	97.21	113.80
1	A	5	PRO	CA-N-CD	-13.71	92.81	112.00
1	C	497	GLN	OE1-CD-NE2	-10.41	112.19	122.60
1	C	502	GLN	OE1-CD-NE2	-10.13	112.47	122.60
1	C	286	GLN	OE1-CD-NE2	-9.95	112.65	122.60
1	B	502	GLN	OE1-CD-NE2	-9.90	112.70	122.60
1	B	286	GLN	OE1-CD-NE2	-9.87	112.73	122.60
1	D	502	GLN	OE1-CD-NE2	-9.79	112.81	122.60
1	A	502	GLN	OE1-CD-NE2	-9.51	113.09	122.60
1	A	286	GLN	OE1-CD-NE2	-9.51	113.09	122.60
1	B	55	GLN	OE1-CD-NE2	-9.33	113.27	122.60
1	A	55	GLN	OE1-CD-NE2	-9.10	113.50	122.60
1	B	303	GLN	OE1-CD-NE2	-9.05	113.55	122.60
1	D	286	GLN	OE1-CD-NE2	-8.88	113.72	122.60
1	C	55	GLN	OE1-CD-NE2	-8.69	113.91	122.60
1	A	111	GLY	N-CA-C	-8.54	103.81	111.67
1	A	423	ASP	CA-C-N	8.54	128.57	119.78
1	A	423	ASP	C-N-CA	8.54	128.57	119.78
1	B	126	LEU	CA-C-N	8.03	129.87	119.84
1	B	126	LEU	C-N-CA	8.03	129.87	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	310	TYR	N-CA-C	7.78	117.44	108.49
1	C	453	ILE	CB-CA-C	-7.70	104.13	111.44
1	D	453	ILE	CB-CA-C	-7.68	104.14	111.44
1	A	281	TYR	CA-C-N	7.49	127.86	119.32
1	A	281	TYR	C-N-CA	7.49	127.86	119.32
1	C	348	ILE	N-CA-C	7.38	117.45	110.74
1	D	502	GLN	CG-CD-NE2	7.19	127.18	116.40
1	C	497	GLN	CG-CD-NE2	7.06	127.00	116.40
1	A	403	VAL	CA-C-N	7.03	127.00	119.76
1	A	403	VAL	C-N-CA	7.03	127.00	119.76
1	B	354	LYS	N-CA-C	-6.93	101.39	110.53
1	B	502	GLN	CG-CD-NE2	6.93	126.79	116.40
1	C	54	VAL	N-CA-C	6.92	118.52	110.62
1	A	453	ILE	CB-CA-C	-6.89	104.89	111.44
1	C	286	GLN	CG-CD-NE2	6.87	126.70	116.40
1	C	423	ASP	CA-C-N	6.78	128.31	119.84
1	C	423	ASP	C-N-CA	6.78	128.31	119.84
1	D	557	LYS	CA-C-N	6.72	126.76	119.90
1	D	557	LYS	C-N-CA	6.72	126.76	119.90
1	D	286	GLN	CG-CD-NE2	6.69	126.44	116.40
1	B	286	GLN	CG-CD-NE2	6.69	126.43	116.40
1	B	281	TYR	CA-C-N	6.63	126.57	119.28
1	B	281	TYR	C-N-CA	6.63	126.57	119.28
1	D	314	GLU	N-CA-C	6.56	120.72	110.17
1	A	126	LEU	CA-C-N	6.49	127.96	119.84
1	A	126	LEU	C-N-CA	6.49	127.96	119.84
1	C	504	ILE	N-CA-C	6.49	117.93	108.58
1	C	502	GLN	CG-CD-NE2	6.49	126.13	116.40
1	B	49	ALA	N-CA-C	-6.45	104.18	111.14
1	A	410	GLY	N-CA-C	-6.43	106.25	115.64
1	C	55	GLN	CG-CD-NE2	6.41	126.02	116.40
1	B	55	GLN	CG-CD-NE2	6.32	125.88	116.40
1	B	504	ILE	N-CA-C	6.29	117.64	108.58
1	A	286	GLN	CG-CD-NE2	6.28	125.81	116.40
1	D	111	GLY	N-CA-C	-6.23	105.94	111.67
1	B	303	GLN	CG-CD-NE2	6.23	125.75	116.40
1	B	453	ILE	CB-CA-C	-6.21	105.54	111.44
1	A	55	GLN	CG-CD-NE2	6.11	125.57	116.40
1	B	201	ILE	N-CA-C	6.01	116.79	110.72
1	A	502	GLN	CG-CD-NE2	5.95	125.33	116.40
1	A	417	GLY	N-CA-C	-5.89	102.94	112.31
1	D	102	MET	N-CA-C	5.89	118.07	108.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	361	LYS	N-CA-C	5.83	118.11	111.11
1	C	354	LYS	N-CA-C	-5.78	102.89	110.53
1	A	359	LEU	N-CA-C	5.67	118.40	111.82
1	B	396	ASN	CA-C-N	5.66	125.33	119.56
1	B	396	ASN	C-N-CA	5.66	125.33	119.56
1	C	407	LYS	N-CA-C	5.66	117.62	110.33
1	A	316	LEU	N-CA-C	5.53	118.47	110.28
1	B	308	ARG	N-CA-C	-5.52	106.33	112.57
1	B	425	VAL	N-CA-C	-5.47	105.76	110.74
1	C	201	ILE	N-CA-C	5.43	116.09	110.82
1	C	281	TYR	CA-C-N	5.42	125.51	119.87
1	C	281	TYR	C-N-CA	5.42	125.51	119.87
1	C	267	GLU	CA-C-N	5.34	125.25	119.85
1	C	267	GLU	C-N-CA	5.34	125.25	119.85
1	D	316	LEU	N-CA-C	5.34	117.97	109.96
1	B	253	LEU	N-CA-C	5.33	117.51	111.11
1	C	396	ASN	CA-C-N	5.28	126.44	119.84
1	C	396	ASN	C-N-CA	5.28	126.44	119.84
1	C	126	LEU	CA-C-N	5.27	126.43	119.84
1	C	126	LEU	C-N-CA	5.27	126.43	119.84
1	C	452	ILE	N-CA-C	5.27	115.89	109.30
1	C	421	THR	N-CA-C	5.20	116.43	108.52
1	C	432	PHE	N-CA-C	5.19	117.02	111.36
1	A	112	LYS	N-CA-C	-5.18	105.64	112.94
1	A	424	PRO	N-CA-C	5.10	119.32	111.21
1	D	368	THR	N-CA-C	-5.08	105.82	111.36
1	B	102	MET	N-CA-C	5.03	116.71	108.76

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	141	0
1	B	4668	0	4676	128	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	4668	0	4676	151	0
1	D	4668	0	4676	110	0
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	5	0
4	C	382	0	0	12	0
4	D	444	0	0	8	0
All	All	20193	0	18704	520	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 14.

All (520) 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:536:LYS:HE2	1:A:554:MET:HE2	1.51	0.92
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:561:VAL:HG12	1:D:562:PRO:HD2	1.65	0.77
1:C:48:MET:HE2	1:C:48:MET:HA	1.65	0.77
1:B:159:THR:OG1	1:B:162:GLU:HG3	1.84	0.76
1:A:205:LYS:HE2	1:A:209:LYS:HZ2	1.51	0.76
1:B:407:LYS:HB2	1:B:411:ALA:O	1.86	0.76
1:A:220:LYS:HE2	1:A:224:TYR:OH	1.85	0.75
1:C:202:ILE:O	1:C:203:THR:HB	1.84	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:367:TRP:NE1	1:D:385:MET:HE2	2.03	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:D:363:PHE:CE1	1:D:385:MET:HE1	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:31:ASN:C	1:A:31:ASN:HD22	2.05	0.64
1:A:93:ILE:HG13	1:A:102:MET:HE2	1.77	0.64
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:D:367:TRP:CE2	1:D:385:MET:HE2	2.32	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:A:466:GLU:CD	1:A:466:GLU:H	2.05	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: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: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:D:31:ASN:C	1:D:31:ASN:HD22	2.08	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:50:TRP:NE1	1:B:54:VAL:HG11	2.17	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:B:161:GLU:CD	1:B:161:GLU:H	2.10	0.58
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:C:336:MET:HE2	1:C:342:LEU:HD21	1.86	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:333:LEU:HD12	1:A:336:MET:HE2	1.88	0.56
1:B:470:VAL:HG13	1:B:471:ILE:HG23	1.87	0.56
1:D:363:PHE:HE1	1:D:385:MET:HE1	1.70	0.56
1:A:469:ASP:HA	1:A:472:LYS:HG3	1.86	0.55
1:B:304:ILE:HD12	1:B:314:GLU:CD	2.32	0.55
1:C:47:PHE:CD2	1:C:48:MET:HE3	2.41	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
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: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:A:202:ILE:O	1:A:203:THR:OG1	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:B:31:ASN:HD22	1:B:31:ASN:C	2.17	0.51
1:C:505:TYR:CE1	1:C:518:PRO:HG3	2.46	0.51
1:A:333:LEU:CD1	1:A:336:MET:HE2	2.41	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:A:466:GLU:CD	1:A:466:GLU:N	2.68	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:47:PHE:HD2	1:C:48:MET:HE3	1.74	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
1:B:336:MET:HE3	1:B:342:LEU:HD11	1.93	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:A:280:ASP:C	1:A:282:PRO:HD3	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:544:GLU:CD	1:C:544:GLU:H	2.19	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:C:48:MET:HE2	1:C:51:VAL:HG21	1.93	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:B:288:ILE:HD11	1:B:336:MET:HE1	1.93	0.50
1:C:187:ARG:NH1	1:C:187:ARG:HG3	2.26	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
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:B:515:GLU:H	1:B:515:GLU:CD	2.20	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:C:313:ASN:CG	4:C:5269:HOH:O	2.55	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: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:47:PHE:CD2	1:B:48:MET:HE2	2.48	0.48
1:B:85:GLY:O	1:B:109:TYR:CE1	2.66	0.48
1:C:101:TYR:HD2	1:C:188:MET:HE3	1.77	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:363:PHE:CZ	1:D:385:MET:HE1	2.48	0.47
1:C:336:MET:HE2	1:C:342:LEU:CD2	2.44	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:363:PHE:CZ	1:D:385:MET:CE	2.98	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
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:210:VAL:C	1:A:212:PRO:HD3	2.40	0.47
1:A:319:SER:HB2	1:A:322:GLU:O	2.14	0.47
1:A:549:GLY:O	1:A:550:PHE:C	2.58	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:451:ARG:NH1	1:D:468:PRO:HG3	2.30	0.46
1:D:93:ILE:HG13	1:D:102:MET:HE2	1.97	0.46
1:D:276:VAL:O	1:D:277:TRP:C	2.59	0.46
1:D:289:ARG:HG3	1:D:348:ILE:CD1	2.40	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:D:336:MET:HE3	1:D:342:LEU:CD2	2.46	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:D:510:ASP:C	1:D:512:LYS:H	2.23	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:B:11:CYS:HA	1:B:28:GLY:O	2.17	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:86:LEU:O	1:C:87:PRO:C	2.58	0.45
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:D:506:MET:HE3	1:D:513:LEU:HG	1.99	0.45
1:C:399:VAL:CG1	1:C:419:GLU:HB3	2.46	0.45
1:D:557:LYS:HA	1:D:558:PRO:HD3	1.78	0.45
1:C:371:LYS:HD2	1:C:371:LYS:C	2.40	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:C:38:TYR:HE1	1:C:163:TYR:HH	1.63	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:188:MET:HB3	4:A:729:HOH:O	2.17	0.44
1:C:366:LYS:NZ	4:C:5115:HOH:O	2.47	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:308:ARG:HG3	1:C:308:ARG:NH1	2.32	0.44
1:B:276:VAL:O	1:B:277:TRP:C	2.58	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
1:D:167:LYS:NZ	4:D:3278:HOH:O	2.50	0.44
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:202:ILE:O	1:B:203:THR:OG1	2.33	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:A:310:TYR:HH	1:A:322:GLU:HG3	1.68	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:D:385:MET:HE3	1:D:385:MET:HB3	1.91	0.42
1:D:520:ASP:CG	1:D:520:ASP:O	2.63	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:27:TYR:CD1	1:B:27:TYR:C	2.98	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:D:549:GLY:O	1:D:550:PHE:C	2.62	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:SER:O	1:A:397:PRO:HD3	2.18	0.42
1:B:29:TYR:C	1:B:29:TYR:CD1	2.98	0.42
1:B:161:GLU:CD	1:B:161:GLU:N	2.76	0.42
1:B:307:SER:C	1:B:309:PHE:H	2.26	0.42
1:D:363:PHE:CE1	1:D:385:MET:CE	3.00	0.42
1:D:555:LYS:HD3	1:D:557:LYS:HE3	2.01	0.42
1:A:34:ASP:OD1	1:A:36:SER:OG	2.29	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:336:MET:HE3	1:A:342:LEU:HD11	2.01	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:A:304:ILE:O	1:A:305:LYS:C	2.63	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:A:226:TYR:CD2	1:A:226:TYR:C	2.98	0.41
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:B:286:GLN:HG3	1:B:288:ILE:HG22	2.01	0.41
1:C:20:GLU:H	1:C:20:GLU:CD	2.28	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
1:A:495:LEU:HG	1:A:546:PHE:CE2	2.55	0.41
1:B:336:MET:HE3	1:B:342:LEU:CD1	2.51	0.41
1:C:405:TYR:CD1	1:C:405:TYR:C	2.97	0.41
1:B:218:LEU:HD23	1:B:218:LEU:HA	1.87	0.41
1:C:246:MET:HE2	1:C:248:PHE:CZ	2.55	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:LEU:O	1:B:67:GLY:N	2.47	0.41
1:B:274:LYS:NZ	4:B:638:HOH:O	2.52	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:90:TYR:CD1	1:B:90:TYR:C	2.99	0.41
1:B:275:TYR:HE1	1:B:352:LYS:HG2	1.86	0.41
1:B:333:LEU:HD12	1:B:336:MET:HE2	2.02	0.41
1:C:405:TYR:HE2	1:C:415:ARG:HG3	1.86	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:B:406:LEU:O	1:B:407:LYS:C	2.62	0.41
1:C:29:TYR:CD1	1:C:29:TYR:C	2.98	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:C:415:ARG:O	1:C:416:LEU:C	2.64	0.41
1:C:18:LYS:NZ	4:C:5210:HOH:O	2.54	0.40
1:C:408:GLU:H	1:C:408:GLU:CD	2.29	0.40
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:C:544:GLU:CD	1:C:544:GLU:N	2.79	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:D:29:TYR:CD1	1:D:29:TYR:C	2.98	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:D:515:GLU:H	1:D:515:GLU:CD	2.28	0.40
1:A:265:TYR:CD1	1:A:265:TYR:C	3.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:25:TRP:CE3	1:C:26:ALA:HB2	2.56	0.40
1:D:27:TYR:CD1	1:D:27:TYR:C	2.99	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%)	10	9
1	B	569/575 (99%)	521 (92%)	44 (8%)	4 (1%)	18	20
1	C	569/575 (99%)	525 (92%)	36 (6%)	8 (1%)	9	7
1	D	569/575 (99%)	536 (94%)	28 (5%)	5 (1%)	14	14
All	All	2276/2300 (99%)	2100 (92%)	152 (7%)	24 (1%)	11	11

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

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Mol	Chain	Res	Type
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
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%)	494 (98%)	8 (2%)	55	70
1	B	502/506 (99%)	493 (98%)	9 (2%)	51	66
1	C	502/506 (99%)	490 (98%)	12 (2%)	43	57
1	D	502/506 (99%)	494 (98%)	8 (2%)	55	70
All	All	2008/2024 (99%)	1971 (98%)	37 (2%)	51	66

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	GLU
1	A	31	ASN
1	A	89	THR
1	A	145	ASP
1	A	185	LEU
1	A	318	SER
1	A	390	TYR
1	A	466	GLU
1	B	16	THR

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Mol	Chain	Res	Type
1	B	20	GLU
1	B	88	ASN
1	B	116	HIS
1	B	145	ASP
1	B	223	ARG
1	B	249	ASP
1	B	504	ILE
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	267	GLU
1	C	288	ILE
1	C	304	ILE
1	C	314	GLU
1	C	409	ASN
1	C	420	GLU
1	C	552	ARG
1	D	20	GLU
1	D	31	ASN
1	D	54	VAL
1	D	113	ARG
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 (36) 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	303	GLN
1	A	380	GLN
1	B	31	ASN
1	B	116	HIS
1	B	171	GLN

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Mol	Chain	Res	Type
1	B	287	HIS
1	B	313	ASN
1	B	396	ASN
1	B	545	ASN
1	B	560	GLN
1	C	31	ASN
1	C	35	HIS
1	C	55	GLN
1	C	72	ASN
1	C	171	GLN
1	C	313	ASN
1	C	344	ASN
1	C	380	GLN
1	C	409	ASN
1	C	545	ASN
1	D	31	ASN
1	D	35	HIS
1	D	55	GLN
1	D	116	HIS
1	D	171	GLN
1	D	284	HIS
1	D	287	HIS
1	D	303	GLN
1	D	409	ASN
1	D	497	GLN
1	D	560	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	3000	-	4,4,4	1.81	2 (50%)	6,6,6	0.87	0
3	SO4	D	3001	-	4,4,4	1.90	1 (25%)	6,6,6	0.81	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	3.20	1.63	1.44
3	D	3000	SO4	O1-S	2.86	1.61	1.44
3	D	3000	SO4	O3-S	-2.16	1.30	1.48

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

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	0.25	35 (6%)	27 31	25, 55, 108, 135	0
1	B	571/575 (99%)	0.09	23 (4%)	42 48	23, 50, 95, 149	0
1	C	571/575 (99%)	-0.03	15 (2%)	57 63	22, 47, 106, 147	0
1	D	571/575 (99%)	-0.25	5 (0%)	81 84	22, 43, 84, 150	0
All	All	2284/2300 (99%)	0.02	78 (3%)	48 55	22, 48, 103, 150	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	309	PHE	4.3
1	A	404	PRO	4.0
1	A	405	TYR	3.8
1	C	400	THR	3.7
1	B	107	LEU	3.6
1	A	310	TYR	3.6
1	D	148	TYR	3.6
1	D	310	TYR	3.6
1	D	309	PHE	3.5
1	C	401	GLY	3.5
1	A	403	VAL	3.4
1	B	309	PHE	3.4
1	A	417	GLY	3.4
1	A	406	LEU	3.3
1	A	148	TYR	3.3
1	A	410	GLY	3.1
1	C	304	ILE	3.0
1	B	111	GLY	3.0
1	B	305	LYS	2.9
1	A	85	GLY	2.9
1	C	421	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	85	GLY	2.8
1	C	399	VAL	2.8
1	A	564	GLY	2.7
1	B	108	GLY	2.7
1	B	312	GLY	2.7
1	B	310	TYR	2.7
1	A	307	SER	2.6
1	A	562	PRO	2.6
1	B	304	ILE	2.6
1	B	406	LEU	2.6
1	B	115	ILE	2.6
1	C	398	ASP	2.6
1	A	86	LEU	2.5
1	A	411	ALA	2.5
1	B	41	GLY	2.5
1	C	545	ASN	2.4
1	B	117	THR	2.4
1	A	399	VAL	2.4
1	C	115	ILE	2.4
1	A	109	TYR	2.4
1	A	81	TRP	2.3
1	C	116	HIS	2.3
1	A	5	PRO	2.3
1	C	310	TYR	2.3
1	B	307	SER	2.3
1	A	565	VAL	2.3
1	A	563	GLY	2.3
1	B	109	TYR	2.3
1	A	17	THR	2.3
1	C	107	LEU	2.2
1	A	93	ILE	2.2
1	A	409	ASN	2.2
1	C	227	ARG	2.2
1	C	308	ARG	2.2
1	A	149	HIS	2.2
1	A	394	ALA	2.2
1	A	413	GLY	2.2
1	D	521	TYR	2.2
1	D	509	VAL	2.2
1	A	560	GLN	2.2
1	B	112	LYS	2.1
1	C	309	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	113	ARG	2.1
1	B	308	ARG	2.1
1	A	110	LYS	2.1
1	A	19	VAL	2.1
1	A	401	GLY	2.1
1	A	15	THR	2.1
1	B	83	ALA	2.1
1	B	151	GLU	2.1
1	A	416	LEU	2.1
1	A	111	GLY	2.1
1	B	421	THR	2.0
1	B	106	CYS	2.0
1	B	149	HIS	2.0
1	A	312	GLY	2.0
1	C	419	GLU	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
3	SO4	D	3001	5/5	0.88	0.15	98,99,102,103	0
3	SO4	D	3000	5/5	0.90	0.11	67,75,77,83	0
2	MG	C	5000	1/1	0.95	0.15	47,47,47,47	0
2	MG	C	5001	1/1	0.96	0.12	53,53,53,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.