



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 05:04 AM UTC

PDB ID : 6WH9 / pdb_00006wh9
Title : Ketoreductase from module 1 of the 6-deoxyerythronolide B synthase (KR1)
in complex with antibody fragment (Fab) 1D10
Authors : Cogan, D.P.; Mathews, I.I.; Khosla, C.
Deposited on : 2020-04-07
Resolution : 2.75 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:

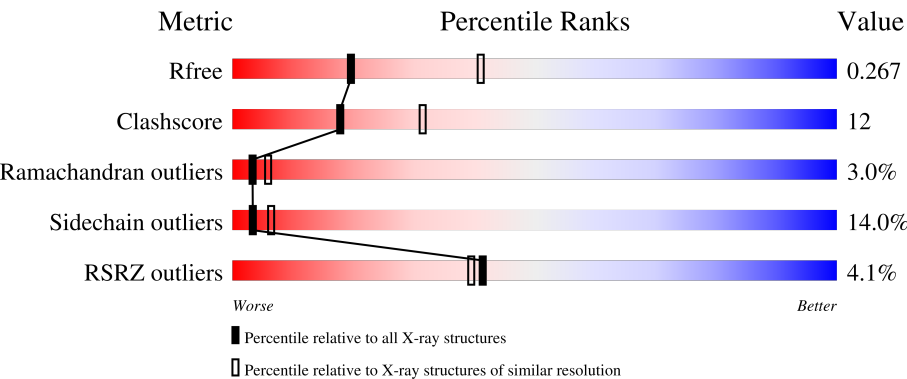
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.75 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	485	5% 64% 22% • 11%
1	D	485	3% 69% 19% • 7%
1	G	485	3% 64% 24% • 9%
2	B	246	% 67% 20% 5% 9%
2	E	246	14% 53% 28% 10% 9%

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Mol	Chain	Length	Quality of chain
2	H	246	 62% 24% 11% 3%
3	C	231	 63% 22% 8% 7%
3	F	231	 65% 23% 6% 3%
3	I	231	 65% 21% 7% 6%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 19434 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 KR1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	439	Total	C	N	O	S	0	0	0
			3237	2023	590	617	7			
1	D	450	Total	C	N	O	S	0	0	0
			3283	2049	593	635	6			
1	A	431	Total	C	N	O	S	0	0	0
			3104	1940	558	599	7			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	1444	GLY	-	expression tag	UNP Q5UNP6
G	1445	SER	-	expression tag	UNP Q5UNP6
G	1446	HIS	-	expression tag	UNP Q5UNP6
G	1447	MET	-	expression tag	UNP Q5UNP6
D	1444	GLY	-	expression tag	UNP Q5UNP6
D	1445	SER	-	expression tag	UNP Q5UNP6
D	1446	HIS	-	expression tag	UNP Q5UNP6
D	1447	MET	-	expression tag	UNP Q5UNP6
A	1444	GLY	-	expression tag	UNP Q5UNP6
A	1445	SER	-	expression tag	UNP Q5UNP6
A	1446	HIS	-	expression tag	UNP Q5UNP6
A	1447	MET	-	expression tag	UNP Q5UNP6

- Molecule 2 is a protein called 1D10 (Fab heavy chain).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	224	Total	C	N	O	S	0	0	0
			1640	1027	275	330	8			
2	B	225	Total	C	N	O	S	0	0	0
			1633	1022	270	333	8			
2	H	219	Total	C	N	O	S	0	0	0
			1613	1013	271	322	7			

- Molecule 3 is a protein called 1D10 (Fab light chain).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	216	Total	C	N	O	S	0	0	0
			1573	997	258	313	5			
3	C	215	Total	C	N	O	S	0	0	0
			1577	999	257	316	5			
3	I	216	Total	C	N	O	S	0	1	0
			1593	1009	259	320	5			

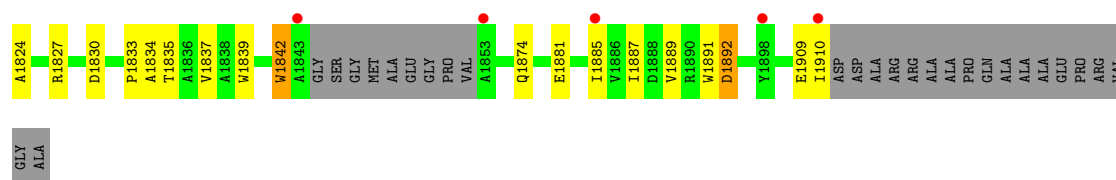
- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	G	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

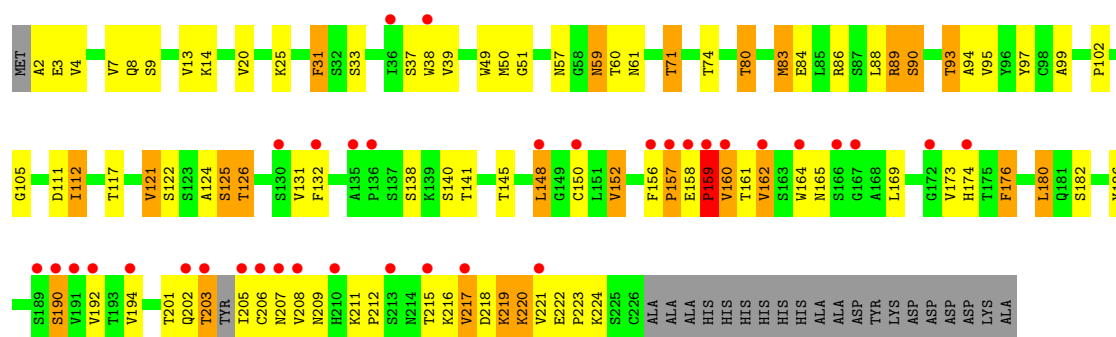
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	14	Total 14	O 14	0	0
5	E	14	Total 14	O 14	0	0
5	F	20	Total 20	O 20	0	0
5	B	13	Total 13	O 13	0	0
5	C	26	Total 26	O 26	0	0
5	H	16	Total 16	O 16	0	0
5	I	23	Total 23	O 23	0	0
5	D	9	Total 9	O 9	0	0
5	A	11	Total 11	O 11	0	0



• Molecule 1: KR1

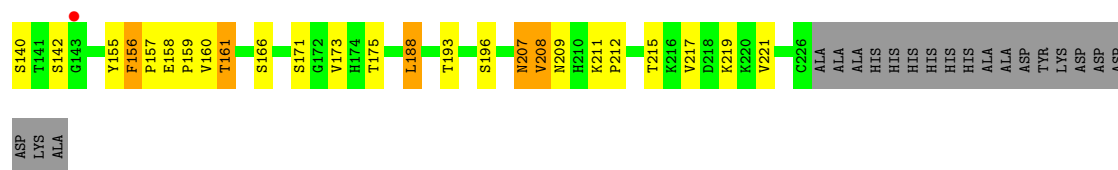


• Molecule 2: 1D10 (Fab heavy chain)

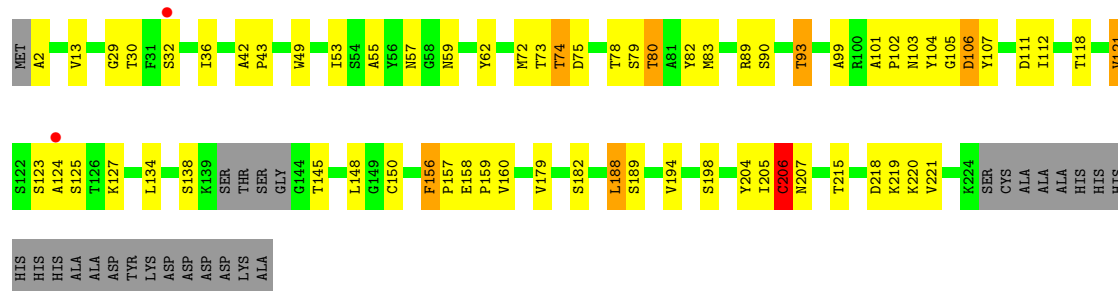


• Molecule 2: 1D10 (Fab heavy chain)

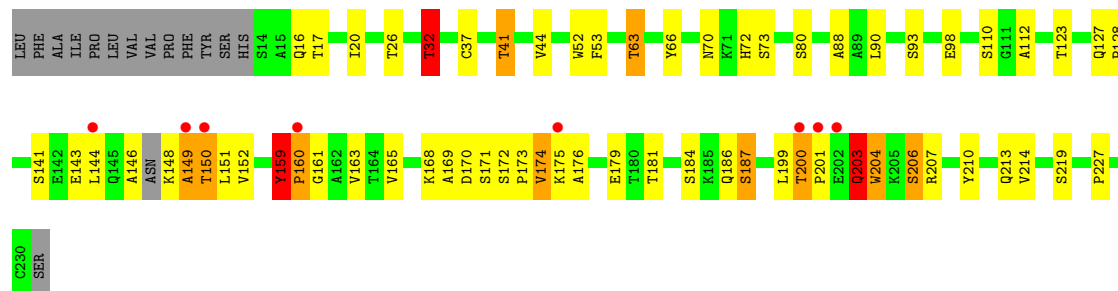




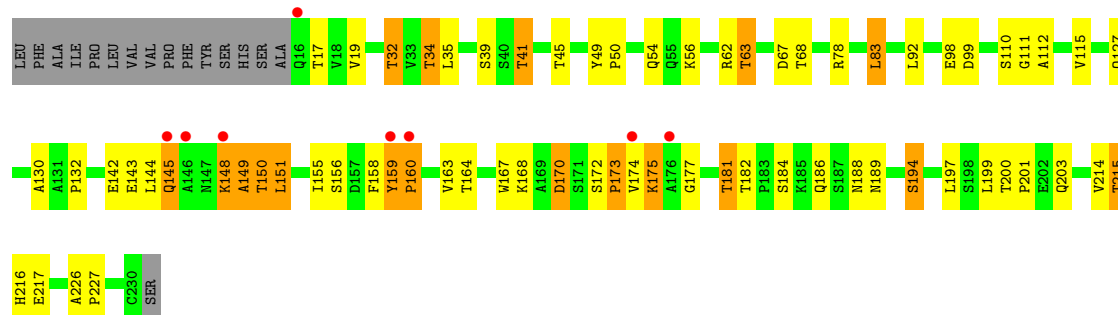
• Molecule 2: 1D10 (Fab heavy chain)



• Molecule 3: 1D10 (Fab light chain)

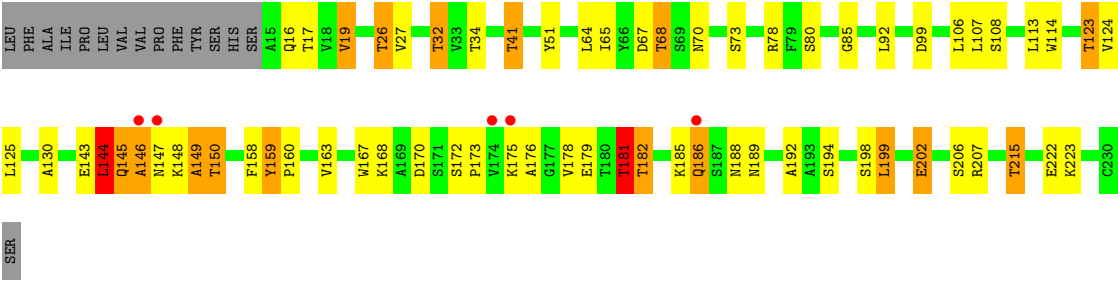


• Molecule 3: 1D10 (Fab light chain)



• Molecule 3: 1D10 (Fab light chain)





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	186.03Å 114.81Å 186.14Å 90.00° 96.53° 90.00°	Depositor
Resolution (Å)	39.59 – 2.75 39.59 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.6 (39.59-2.75) 99.6 (39.59-2.75)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.228 , 0.271 0.229 , 0.267	Depositor DCC
R_{free} test set	5043 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	83.7	Xtriage
Anisotropy	0.336	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 67.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	19434	wwPDB-VP
Average B, all atoms (Å ²)	107.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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

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	1.06	0/3156	1.53	7/4311 (0.2%)
1	D	1.04	0/3340	1.50	3/4558 (0.1%)
1	G	1.03	0/3294	1.47	1/4490 (0.0%)
2	B	1.06	0/1672	1.41	4/2291 (0.2%)
2	E	1.07	0/1676	1.42	1/2286 (0.0%)
2	H	1.07	0/1650	1.39	1/2253 (0.0%)
3	C	1.06	1/1620 (0.1%)	1.43	7/2223 (0.3%)
3	F	1.06	1/1615 (0.1%)	1.39	2/2215 (0.1%)
3	I	1.07	0/1636	1.40	4/2244 (0.2%)
All	All	1.05	2/19659 (0.0%)	1.45	30/26871 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	159	TYR	C-N	6.86	1.49	1.33
3	F	149	ALA	C-O	5.76	1.31	1.24

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	34	THR	CB-CA-C	8.06	122.56	110.14
3	C	159	TYR	CA-C-N	7.01	128.61	119.84
3	C	159	TYR	C-N-CA	7.01	128.61	119.84
3	C	159	TYR	N-CA-CB	6.18	121.37	110.37
1	A	1536	GLU	CB-CA-C	-6.10	107.84	115.89
1	D	1762	ASP	CA-CB-CG	6.08	118.68	112.60
3	C	215	THR	CB-CA-C	6.07	120.24	110.16
3	C	170	ASP	CA-CB-CG	5.89	118.49	112.60
2	E	176	PHE	CB-CA-C	5.85	118.68	109.37
2	H	206	CYS	N-CA-CB	5.85	118.56	109.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1805	PHE	CA-CB-CG	5.83	119.63	113.80
2	B	207	ASN	CA-C-N	-5.58	114.92	122.91
2	B	207	ASN	C-N-CA	-5.58	114.92	122.91
1	A	1646	TYR	CA-C-N	5.51	125.40	121.65
1	A	1646	TYR	C-N-CA	5.51	125.40	121.65
2	B	116	GLY	CA-C-O	-5.50	117.45	122.24
3	I	181	THR	CA-C-N	5.19	128.03	120.51
3	I	181	THR	C-N-CA	5.19	128.03	120.51
1	G	1460	ARG	CB-CA-C	5.18	116.18	108.87
3	F	159	TYR	N-CA-CB	5.18	119.58	110.37
1	D	1672	GLY	CA-C-N	5.18	125.72	119.98
1	D	1672	GLY	C-N-CA	5.18	125.72	119.98
2	B	173	VAL	N-CA-CB	5.16	116.15	110.53
1	A	1791	ASP	CA-CB-CG	5.10	117.70	112.60
3	I	202	GLU	N-CA-C	-5.08	105.44	111.69
3	I	123	THR	CB-CA-C	5.07	118.10	109.84
3	C	151	LEU	N-CA-C	-5.06	101.06	109.46
1	A	1448	ASP	CA-C-N	5.05	127.75	120.38
1	A	1448	ASP	C-N-CA	5.05	127.75	120.38
3	F	32	THR	CA-CB-OG1	-5.03	102.06	109.60

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	3104	0	3008	58	0
1	D	3283	0	3191	60	0
1	G	3237	0	3184	71	0
2	B	1633	0	1543	34	0
2	E	1640	0	1589	78	0
2	H	1613	0	1561	50	0
3	C	1577	0	1506	61	0
3	F	1573	0	1500	38	0
3	I	1593	0	1525	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
4	E	5	0	0	0	0
4	F	5	0	0	0	0
4	G	5	0	0	0	0
5	A	11	0	0	1	0
5	B	13	0	0	0	0
5	C	26	0	0	2	0
5	D	9	0	0	0	0
5	E	14	0	0	0	0
5	F	20	0	0	3	0
5	G	14	0	0	3	0
5	H	16	0	0	0	0
5	I	23	0	0	1	0
All	All	19434	0	18607	465	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 12.

All (465) 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:1760:THR:HB	1:A:1762:ASP:OD1	1.60	1.00
2:E:90:SER:O	2:E:93:THR:HG23	1.66	0.96
2:B:89:ARG:HD2	2:B:90:SER:H	1.38	0.89
2:E:20:VAL:HG23	2:E:88:LEU:HD11	1.53	0.89
3:C:186:GLN:NE2	3:C:188:ASN:HD22	1.75	0.83
2:H:101:ALA:HB1	2:H:105:GLY:HA3	1.60	0.82
1:A:1764:LEU:HD21	1:A:1769:ILE:HD11	1.62	0.82
3:C:160:PRO:HB2	3:C:216:HIS:NE2	1.93	0.82
3:F:110:SER:HB3	1:D:1699:SER:HB2	1.62	0.81
3:C:159:TYR:HB3	3:C:160:PRO:HD3	1.61	0.80
3:F:168:LYS:HA	3:F:173:PRO:HD2	1.65	0.78
3:F:149:ALA:O	3:F:150:THR:OG1	2.04	0.76
3:C:160:PRO:HG2	3:C:216:HIS:CE1	2.20	0.76
2:B:156:PHE:HB3	2:B:157:PRO:HD3	1.67	0.75
2:H:78:THR:HG23	2:H:80:THR:HG23	1.66	0.75
3:I:159:TYR:O	3:I:160:PRO:C	2.30	0.75
3:I:168:LYS:HA	3:I:173:PRO:HD2	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:159:TYR:O	3:F:160:PRO:C	2.30	0.75
2:H:102:PRO:HD3	2:H:111:ASP:HB2	1.73	0.71
2:H:89:ARG:O	2:H:121:VAL:HG21	1.91	0.70
3:C:173:PRO:O	3:C:175:LYS:N	2.24	0.70
1:G:1451:SER:HA	1:G:1454:ARG:HD3	1.74	0.70
1:D:1597:ARG:NH1	1:D:1803:SER:O	2.25	0.70
1:G:1755:THR:HG22	5:G:2108:HOH:O	1.91	0.70
3:C:181:THR:HG22	3:C:182:THR:O	1.92	0.69
1:G:1713:LEU:HD13	1:G:1720:THR:HG21	1.72	0.69
2:E:89:ARG:HD3	2:E:90:SER:H	1.58	0.69
2:E:162:VAL:HG23	2:E:208:VAL:HG22	1.75	0.69
1:G:1699:SER:OG	3:C:110:SER:HB3	1.94	0.68
3:I:146:ALA:O	3:I:148:LYS:N	2.25	0.68
2:H:62:TYR:HE1	2:H:72:MET:HG2	1.59	0.68
1:G:1726:ASP:OD2	3:C:45:THR:HG23	1.94	0.68
3:C:144:LEU:CD2	3:C:148:LYS:CB	2.72	0.67
3:C:17:THR:OG1	3:C:41:THR:HG21	1.95	0.67
2:H:90:SER:HA	2:H:121:VAL:CG2	2.25	0.67
1:G:1764:LEU:HD21	1:G:1769:ILE:HD11	1.76	0.66
2:B:126:THR:HA	2:B:156:PHE:HB3	1.77	0.66
2:E:173:VAL:HG22	2:E:192:VAL:HG22	1.78	0.66
3:C:110:SER:OG	3:C:111:GLY:N	2.25	0.66
3:I:167:TRP:O	3:I:173:PRO:HD2	1.96	0.65
1:G:1552:THR:HG22	5:G:2101:HOH:O	1.96	0.65
3:C:167:TRP:O	3:C:173:PRO:HD2	1.96	0.65
3:F:53:PHE:CE1	3:F:63:THR:HB	2.32	0.65
3:C:186:GLN:HE22	3:C:188:ASN:HD22	1.44	0.65
2:B:93:THR:HG22	2:B:121:VAL:H	1.62	0.65
2:H:90:SER:O	2:H:93:THR:HG23	1.97	0.64
1:D:1583:ARG:NH1	1:D:1830:ASP:OD1	2.26	0.64
2:B:161:THR:HG22	2:B:209:ASN:HB3	1.79	0.64
3:I:143:GLU:O	3:I:145:GLN:N	2.27	0.64
1:A:1583:ARG:NH1	1:A:1830:ASP:OD1	2.31	0.63
3:F:53:PHE:CD1	3:F:63:THR:HB	2.33	0.63
2:B:188:LEU:C	2:B:188:LEU:HD12	2.23	0.63
2:H:90:SER:HA	2:H:121:VAL:HG23	1.79	0.63
2:H:156:PHE:HB3	2:H:157:PRO:HD3	1.81	0.63
2:E:169:LEU:HD22	2:E:192:VAL:HG11	1.80	0.63
2:H:75:ASP:OD2	2:H:78:THR:HG22	1.98	0.63
2:E:38:TRP:HB3	2:E:50:MET:HE3	1.81	0.62
1:G:1613:VAL:HG21	1:G:1621:LEU:HD22	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1475:LEU:HD23	1:A:1525:VAL:HG21	1.81	0.62
2:H:101:ALA:CB	2:H:105:GLY:HA3	2.29	0.62
3:C:160:PRO:CB	3:C:216:HIS:NE2	2.62	0.62
1:A:1597:ARG:HD2	1:A:1637:GLN:OE1	2.00	0.62
3:C:143:GLU:C	3:C:145:GLN:H	2.08	0.61
2:E:211:LYS:HB2	2:E:212:PRO:HD3	1.83	0.61
3:I:144:LEU:HA	3:I:148:LYS:CB	2.31	0.61
3:I:67:ASP:OD2	1:A:1774:ARG:NH2	2.33	0.61
3:I:206:SER:OG	3:I:207:ARG:N	2.31	0.61
2:E:25:LYS:HG3	2:E:80:THR:HG22	1.84	0.60
2:E:202:GLN:HG2	2:E:203:THR:H	1.66	0.60
1:G:1839:TRP:CD2	1:G:1842:TRP:HZ3	2.19	0.60
2:E:93:THR:HG22	2:E:121:VAL:H	1.66	0.60
3:I:32:THR:HA	3:I:92:LEU:O	2.02	0.60
2:B:89:ARG:HD2	2:B:90:SER:N	2.12	0.60
2:H:55:ALA:HA	2:H:74:THR:HG21	1.83	0.60
1:D:1458:GLU:OE1	1:D:1460:ARG:NH1	2.35	0.60
1:G:1483:ALA:O	1:G:1486:THR:N	2.33	0.59
2:E:57:ASN:OD1	2:E:59:ASN:HB2	2.02	0.59
1:D:1684:TRP:CE3	1:D:1685:LEU:HD23	2.38	0.59
3:I:143:GLU:C	3:I:145:GLN:H	2.10	0.59
3:I:143:GLU:OE1	3:I:150:THR:HG23	2.02	0.59
2:E:164:TRP:CE2	2:E:192:VAL:HG23	2.37	0.59
2:H:2:ALA:CB	2:H:103:ASN:H	2.16	0.59
1:A:1572:THR:HG21	1:A:1593:TRP:HE1	1.67	0.59
2:B:83:MET:SD	2:B:83:MET:C	2.86	0.58
1:G:1611:VAL:HG23	1:G:1640:LEU:HD13	1.85	0.58
3:C:155:ILE:HG22	3:C:158:PHE:CE1	2.38	0.58
2:E:71:THR:OG1	2:E:86:ARG:NH1	2.37	0.58
1:G:1813:TYR:O	1:G:1817:ASN:ND2	2.35	0.58
3:C:132:PRO:HB3	3:C:158:PHE:CD1	2.39	0.58
2:E:162:VAL:CG1	2:E:162:VAL:O	2.51	0.57
3:C:181:THR:CG2	3:C:182:THR:O	2.51	0.57
3:C:144:LEU:HD23	3:C:148:LYS:CB	2.34	0.57
3:F:168:LYS:CA	3:F:173:PRO:HD2	2.35	0.57
3:I:168:LYS:HA	3:I:173:PRO:CD	2.35	0.57
1:D:1460:ARG:HG3	1:D:1909:GLU:OE1	2.04	0.57
1:D:1589:HIS:HA	1:D:1592:LEU:HD12	1.87	0.57
1:G:1683:ARG:O	1:G:1687:ARG:HG2	2.04	0.57
1:G:1581:PHE:HA	1:D:1462:THR:HG22	1.85	0.57
2:E:164:TRP:CD1	2:E:192:VAL:HG22	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:26:THR:HG22	3:F:123:THR:OG1	2.04	0.57
1:G:1731:GLU:OE1	1:G:1734:ARG:NH2	2.38	0.56
1:G:1814:ALA:HB3	1:G:1815:PRO:HD3	1.86	0.56
2:E:132:PHE:CE1	3:F:143:GLU:HA	2.40	0.56
1:D:1474:TRP:CZ2	1:D:1629:VAL:HG11	2.41	0.56
1:D:1539:PRO:O	1:D:1540:GLU:O	2.24	0.56
1:A:1620:GLU:CD	1:A:1620:GLU:H	2.13	0.56
1:A:1764:LEU:HD21	1:A:1769:ILE:CD1	2.35	0.56
3:I:186[B]:GLN:HE21	3:I:192:ALA:HB2	1.71	0.56
1:D:1814:ALA:HB3	1:D:1815:PRO:HD3	1.87	0.56
2:E:8:GLN:NE2	2:E:117:THR:HG23	2.21	0.56
3:F:32:THR:HG21	5:F:418:HOH:O	2.05	0.56
1:D:1684:TRP:CE3	1:D:1685:LEU:CD2	2.89	0.56
2:B:50:MET:HE1	2:B:83:MET:CE	2.36	0.56
2:B:156:PHE:O	2:B:157:PRO:C	2.48	0.56
3:C:160:PRO:CG	3:C:216:HIS:CE1	2.89	0.56
3:F:200:THR:CB	3:F:201:PRO:HD3	2.36	0.55
3:C:163:VAL:HG12	3:C:216:HIS:HB2	1.87	0.55
1:G:1693:LEU:HB2	1:G:1720:THR:HG22	1.88	0.55
1:G:1726:ASP:OD1	1:G:1728:THR:OG1	2.22	0.55
2:E:222:GLU:CB	2:E:223:PRO:CD	2.84	0.55
1:A:1740:ILE:HD12	1:A:1746:LEU:HB2	1.89	0.55
1:G:1625:LEU:O	1:G:1628:VAL:HG12	2.07	0.55
2:H:101:ALA:HB1	2:H:105:GLY:CA	2.35	0.55
1:D:1813:TYR:O	1:D:1817:ASN:ND2	2.39	0.55
2:E:160:VAL:HG13	2:E:208:VAL:HG13	1.88	0.55
1:A:1688:ARG:HH21	1:A:1874:GLN:NE2	2.04	0.55
1:G:1534:VAL:HG13	1:G:1573:GLU:CD	2.33	0.54
3:F:159:TYR:HB3	3:F:160:PRO:HD3	1.89	0.54
1:G:1597:ARG:NH1	1:G:1803:SER:O	2.41	0.54
2:E:111:ASP:OD1	3:F:72:HIS:NE2	2.40	0.54
1:A:1635:GLU:HB3	1:A:1638:LEU:HD21	1.90	0.54
1:A:1650:TRP:CD1	1:A:1906:LEU:HD21	2.42	0.54
3:C:148:LYS:H	3:C:201:PRO:HD3	1.73	0.54
1:D:1770:GLU:OE2	1:D:1774:ARG:NH1	2.40	0.54
1:A:1688:ARG:NH2	1:A:1874:GLN:NE2	2.55	0.54
2:H:104:TYR:CB	1:A:1512:ARG:HH12	2.21	0.54
3:I:159:TYR:HB3	3:I:160:PRO:HD3	1.89	0.54
2:E:8:GLN:HE21	2:E:117:THR:HG23	1.72	0.54
2:H:156:PHE:O	2:H:157:PRO:C	2.51	0.54
2:E:164:TRP:HE1	2:E:173:VAL:HG13	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1474:TRP:CH2	1:D:1629:VAL:HG11	2.42	0.54
1:G:1528:VAL:HG11	1:G:1559:MET:SD	2.48	0.53
3:C:160:PRO:CG	3:C:216:HIS:NE2	2.71	0.53
1:A:1776:LYS:HG2	1:A:1820:LEU:HD11	1.90	0.53
2:E:9:SER:O	2:E:117:THR:HG22	2.08	0.53
3:F:204:TRP:CZ2	3:F:227:PRO:HA	2.43	0.53
1:A:1744:VAL:HG13	1:A:1744:VAL:O	2.08	0.53
1:D:1515:LEU:HD23	1:D:1558:ALA:CB	2.38	0.53
1:D:1466:GLU:HB2	1:D:1631:GLY:HA2	1.91	0.53
2:H:148:LEU:HD11	2:H:221:VAL:HG12	1.90	0.53
2:H:179:VAL:HG21	3:I:179:GLU:HB3	1.88	0.53
2:H:101:ALA:CB	2:H:106:ASP:H	2.21	0.53
2:E:157:PRO:HB3	2:E:212:PRO:HD2	1.89	0.53
3:C:78:ARG:NH1	3:C:99:ASP:OD1	2.42	0.53
2:B:113:TRP:HE1	3:C:63:THR:HG22	1.73	0.53
3:I:17:THR:OG1	3:I:41:THR:HG21	2.09	0.53
1:G:1459:TRP:CZ2	1:G:1576:VAL:HG11	2.44	0.53
2:E:162:VAL:HG11	2:E:190:SER:CB	2.38	0.52
1:D:1540:GLU:C	1:D:1540:GLU:OE1	2.52	0.52
2:E:180:LEU:HB3	2:E:186:TYR:CE1	2.45	0.52
2:B:42:ALA:O	2:B:43:PRO:C	2.52	0.52
3:C:130:ALA:HB3	3:C:159:TYR:H	1.74	0.52
1:G:1696:VAL:HG11	1:G:1736:LEU:HD21	1.91	0.52
1:G:1747:SER:O	1:G:1793:THR:N	2.38	0.52
3:C:56:LYS:HE2	3:C:98:GLU:O	2.09	0.52
3:F:110:SER:HB3	1:D:1699:SER:CB	2.34	0.52
3:I:108:SER:OG	1:A:1698:ARG:NH1	2.43	0.52
2:E:164:TRP:HB2	2:E:169:LEU:O	2.10	0.52
2:B:93:THR:CG2	2:B:121:VAL:H	2.22	0.52
2:H:62:TYR:CE1	2:H:72:MET:HG2	2.44	0.52
1:A:1474:TRP:CB	5:A:2110:HOH:O	2.58	0.51
1:G:1839:TRP:CD2	1:G:1842:TRP:CZ3	2.97	0.51
2:E:169:LEU:CD2	2:E:192:VAL:HG11	2.40	0.51
1:D:1461:PRO:O	1:D:1462:THR:HG23	2.11	0.51
1:D:1557:GLN:NE2	1:D:1764:LEU:O	2.42	0.51
1:G:1551:ASP:O	1:G:1555:LEU:HB2	2.10	0.51
2:B:40:ARG:NH2	2:B:92:ASP:OD1	2.44	0.51
2:H:102:PRO:HD3	2:H:111:ASP:CB	2.38	0.51
1:A:1505:VAL:O	1:A:1518:ARG:NH1	2.40	0.51
1:A:1734:ARG:HD3	1:A:1786:LEU:HD21	1.91	0.51
1:G:1538:GLU:O	1:G:1540:GLU:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:149:ALA:C	3:F:150:THR:HG1	2.16	0.51
2:H:158:GLU:N	2:H:159:PRO:CD	2.74	0.51
1:D:1464:ALA:HA	1:D:1633:ALA:HB2	1.93	0.51
1:G:1681:ILE:O	1:G:1685:LEU:HB2	2.11	0.51
1:G:1482:THR:O	1:G:1483:ALA:HB3	2.11	0.50
2:H:83:MET:SD	2:H:83:MET:C	2.94	0.50
2:H:194:VAL:HG11	2:H:204:TYR:CE1	2.46	0.50
1:D:1891:TRP:O	1:D:1892:ASP:C	2.54	0.50
2:H:2:ALA:HB2	2:H:102:PRO:HB2	1.92	0.50
1:A:1814:ALA:HB3	1:A:1815:PRO:HD3	1.93	0.50
2:H:124:ALA:HB1	2:H:156:PHE:CG	2.47	0.50
1:G:1555:LEU:HD13	1:G:1568:LEU:HD11	1.93	0.50
1:A:1573:GLU:HA	1:A:1613:VAL:O	2.11	0.50
3:F:159:TYR:O	3:F:161:GLY:N	2.44	0.50
2:E:131:VAL:HG21	2:E:217:VAL:HG11	1.92	0.50
3:F:32:THR:HG22	5:F:403:HOH:O	2.11	0.50
3:C:155:ILE:HG22	3:C:158:PHE:HE1	1.77	0.50
3:C:181:THR:HB	3:C:194:SER:H	1.77	0.50
2:E:164:TRP:CD1	2:E:192:VAL:CG2	2.94	0.49
2:E:209:ASN:HA	2:E:216:LYS:HA	1.94	0.49
2:E:83:MET:SD	2:E:83:MET:C	2.95	0.49
2:E:124:ALA:O	2:E:125:SER:HB2	2.12	0.49
2:E:148:LEU:HD21	2:E:194:VAL:HG13	1.94	0.49
2:B:125:SER:O	2:B:126:THR:C	2.55	0.49
1:A:1490:ALA:O	1:A:1494:LEU:HD23	2.12	0.49
2:E:20:VAL:O	2:E:84:GLU:HA	2.13	0.49
2:B:83:MET:HE1	2:B:85:LEU:HB2	1.94	0.49
1:A:1635:GLU:OE1	1:A:1905:ARG:HB2	2.13	0.49
3:I:19:VAL:CG1	3:I:107:LEU:HD12	2.43	0.49
1:G:1774:ARG:NH2	3:C:67:ASP:OD1	2.46	0.49
1:A:1707:GLY:O	1:A:1710:VAL:HG12	2.13	0.49
1:A:1764:LEU:HD23	1:A:1764:LEU:C	2.38	0.49
1:G:1530:SER:CB	5:G:2101:HOH:O	2.60	0.48
2:E:95:VAL:HG23	2:E:97:TYR:CE2	2.48	0.48
3:C:143:GLU:CB	5:C:409:HOH:O	2.61	0.48
3:C:159:TYR:O	3:C:159:TYR:CD1	2.66	0.48
1:D:1489:ALA:CB	1:D:1618:VAL:CG1	2.91	0.48
2:E:164:TRP:CE2	2:E:192:VAL:CG2	2.97	0.48
3:C:143:GLU:C	3:C:145:GLN:N	2.71	0.48
2:B:158:GLU:O	2:B:158:GLU:OE2	2.32	0.48
1:D:1620:GLU:CD	1:D:1620:GLU:H	2.21	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1559:MET:HE1	1:G:1568:LEU:HB2	1.95	0.48
3:F:127:GLN:HB2	3:F:128:PRO:HD2	1.96	0.48
3:I:215:THR:HG23	5:I:311:HOH:O	2.13	0.48
1:D:1807:ALA:HB3	1:D:1810:LEU:HD12	1.95	0.48
2:E:131:VAL:HG12	2:E:219:LYS:HD3	1.96	0.48
3:F:17:THR:HG23	3:F:41:THR:CG2	2.44	0.48
1:D:1837:VAL:HG11	1:D:1839:TRP:CZ2	2.48	0.48
2:H:158:GLU:N	2:H:159:PRO:HD2	2.29	0.48
3:C:188:ASN:O	3:C:189:ASN:HB2	2.13	0.47
3:F:159:TYR:CD1	3:F:159:TYR:C	2.90	0.47
3:I:222:GLU:HG3	3:I:222:GLU:O	2.13	0.47
1:A:1694:LEU:HD21	1:A:1736:LEU:HD11	1.94	0.47
3:I:149:ALA:HB1	3:I:199:LEU:CD2	2.45	0.47
2:B:110:PHE:O	3:C:63:THR:HG21	2.14	0.47
2:H:2:ALA:CB	2:H:103:ASN:N	2.76	0.47
2:H:188:LEU:C	2:H:188:LEU:HD23	2.40	0.47
3:I:78:ARG:NH2	3:I:99:ASP:OD1	2.48	0.47
2:E:156:PHE:H	2:E:157:PRO:CD	2.27	0.47
2:B:89:ARG:O	2:B:121:VAL:HG21	2.14	0.47
2:E:132:PHE:CD1	3:F:143:GLU:HA	2.49	0.47
2:E:156:PHE:N	2:E:157:PRO:CD	2.78	0.47
2:H:62:TYR:HE1	2:H:72:MET:CG	2.25	0.47
2:H:205:ILE:HD12	2:H:207:ASN:HD21	1.78	0.47
1:D:1471:ASP:OD1	1:D:1471:ASP:C	2.57	0.47
3:F:174:VAL:O	3:F:176:ALA:O	2.32	0.47
3:C:19:VAL:HG21	3:C:115:VAL:HG13	1.97	0.47
3:C:78:ARG:HG3	3:C:92:LEU:CD1	2.45	0.47
2:H:134:LEU:HG	2:H:150:CYS:HA	1.96	0.47
3:I:130:ALA:O	3:I:158:PHE:HA	2.15	0.47
1:A:1545:ALA:O	1:A:1546:LEU:C	2.57	0.47
2:E:159:PRO:HG2	2:E:212:PRO:HD3	1.97	0.47
1:G:1799:SER:OG	1:G:1817:ASN:HB3	2.15	0.47
1:G:1837:VAL:HG11	1:G:1839:TRP:CZ2	2.49	0.47
2:E:162:VAL:HG11	2:E:190:SER:OG	2.15	0.47
2:B:102:PRO:HD3	2:B:111:ASP:HB2	1.95	0.47
2:B:188:LEU:C	2:B:188:LEU:CD1	2.88	0.47
3:F:17:THR:HG23	3:F:41:THR:HG23	1.96	0.46
3:I:168:LYS:CA	3:I:173:PRO:HD2	2.42	0.46
3:I:41:THR:HB	1:A:1702:ASP:OD2	2.16	0.46
3:I:149:ALA:HB1	3:I:199:LEU:HD23	1.97	0.46
2:E:220:LYS:HD3	2:E:220:LYS:C	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:186:GLN:HG3	3:F:187:SER:N	2.30	0.46
1:G:1839:TRP:CG	1:G:1842:TRP:HZ3	2.34	0.46
1:A:1529:LEU:HD11	1:A:1571:VAL:HG13	1.97	0.46
2:H:89:ARG:O	2:H:121:VAL:CG2	2.60	0.46
2:H:101:ALA:HB2	2:H:106:ASP:H	1.80	0.46
3:C:78:ARG:HG3	3:C:92:LEU:HD12	1.98	0.46
1:D:1718:ALA:O	1:D:1720:THR:HG23	2.16	0.46
2:E:89:ARG:O	2:E:121:VAL:HG21	2.16	0.46
2:E:202:GLN:HG2	2:E:203:THR:N	2.31	0.46
1:A:1475:LEU:O	1:A:1528:VAL:HA	2.15	0.46
1:G:1552:THR:HG21	1:G:1592:LEU:CD1	2.45	0.46
2:E:206:CYS:O	2:E:218:ASP:HA	2.15	0.46
2:B:52:TRP:HE1	3:C:112:ALA:HB1	1.81	0.46
3:C:159:TYR:CD1	3:C:159:TYR:C	2.86	0.46
1:G:1598:VAL:HG22	1:G:1598:VAL:O	2.16	0.45
2:H:205:ILE:HA	2:H:219:LYS:O	2.16	0.45
1:G:1459:TRP:CZ2	1:G:1576:VAL:CG1	2.99	0.45
1:G:1742:ASP:OD1	1:G:1742:ASP:N	2.50	0.45
2:E:207:ASN:OD1	2:E:207:ASN:N	2.50	0.45
2:B:90:SER:HA	2:B:121:VAL:HG23	1.98	0.45
2:H:93:THR:HG22	2:H:121:VAL:H	1.82	0.45
2:E:14:LYS:HG3	2:E:20:VAL:HG22	1.98	0.45
3:F:169:ALA:HB1	3:F:207:ARG:HG3	1.97	0.45
2:H:53:ILE:HD13	2:H:73:THR:CA	2.46	0.45
1:D:1464:ALA:HB2	1:D:1633:ALA:HB3	1.98	0.45
2:B:66:LEU:O	2:B:67:GLN:C	2.59	0.45
2:E:105:GLY:O	1:D:1768:ARG:HD2	2.17	0.45
3:F:199:LEU:HD11	3:F:210:TYR:CE2	2.51	0.45
3:C:32:THR:HG22	5:C:403:HOH:O	2.16	0.45
1:D:1839:TRP:HB3	1:D:1842:TRP:HZ3	1.82	0.45
1:A:1776:LYS:NZ	1:A:1798:PHE:O	2.49	0.45
2:E:152:VAL:HG11	2:E:160:VAL:HG11	1.98	0.45
2:H:2:ALA:CB	2:H:102:PRO:HB2	2.47	0.45
3:I:181:THR:HG23	3:I:182:THR:O	2.17	0.45
2:H:73:THR:HG22	2:H:82:TYR:HB2	1.98	0.45
2:H:124:ALA:HB1	2:H:156:PHE:CD1	2.52	0.45
3:I:26:THR:HA	3:I:123:THR:O	2.17	0.45
1:A:1457:ILE:HG12	1:A:1885:ILE:HD11	1.98	0.45
2:E:164:TRP:NE1	2:E:173:VAL:HG13	2.32	0.45
2:B:131:VAL:HG11	2:B:208:VAL:HG11	1.98	0.45
3:C:68:THR:HG23	3:C:83:LEU:HD13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:49:TYR:N	3:C:50:PRO:HD3	2.32	0.45
3:C:160:PRO:HD2	3:C:216:HIS:NE2	2.32	0.45
1:A:1770:GLU:OE1	1:A:1774:ARG:NH1	2.50	0.45
1:G:1702:ASP:OD2	3:C:41:THR:HG22	2.16	0.44
1:A:1604:PRO:HB3	1:A:1902:ARG:HD2	1.98	0.44
2:E:162:VAL:O	2:E:162:VAL:HG12	2.17	0.44
2:B:126:THR:HA	2:B:157:PRO:HD3	1.99	0.44
1:G:1731:GLU:OE1	1:G:1731:GLU:HA	2.18	0.44
2:E:161:THR:O	2:E:208:VAL:HA	2.16	0.44
2:H:49:TRP:CZ3	3:I:113:LEU:HD12	2.53	0.44
1:G:1545:ALA:O	1:G:1546:LEU:C	2.60	0.44
1:G:1613:VAL:HG21	1:G:1621:LEU:CD2	2.45	0.44
3:F:203:GLN:OE1	3:F:203:GLN:HA	2.10	0.44
1:A:1885:ILE:HG22	1:A:1887:ILE:HG22	2.00	0.44
1:D:1790:LEU:HB3	1:D:1792:LEU:HD21	2.00	0.44
1:A:1891:TRP:O	1:A:1892:ASP:C	2.60	0.44
1:G:1614:PRO:O	1:G:1615:ALA:C	2.61	0.44
1:G:1870:CYS:O	1:G:1873:LEU:HB3	2.18	0.44
3:C:149:ALA:HB2	3:C:199:LEU:O	2.18	0.44
2:E:20:VAL:CG2	2:E:88:LEU:HD11	2.38	0.44
3:I:185:LYS:CE	3:I:189:ASN:OD1	2.66	0.44
2:B:158:GLU:N	2:B:159:PRO:HD2	2.32	0.43
3:I:78:ARG:HH21	3:I:99:ASP:CG	2.26	0.43
1:A:1480:ALA:HB2	1:A:1505:VAL:HG21	2.00	0.43
1:A:1613:VAL:HG21	1:A:1621:LEU:HD13	2.00	0.43
1:A:1776:LYS:CG	1:A:1820:LEU:HD11	2.48	0.43
1:G:1757:ASP:CG	1:G:1768:ARG:HE	2.26	0.43
3:C:168:LYS:HA	3:C:173:PRO:HD2	2.00	0.43
2:H:206:CYS:O	2:H:218:ASP:HA	2.17	0.43
1:A:1475:LEU:HD12	1:A:1504:LEU:HB2	1.99	0.43
1:A:1586:ASN:HB3	1:A:1589:HIS:CD2	2.53	0.43
2:E:164:TRP:NE1	2:E:192:VAL:HG22	2.33	0.43
2:H:57:ASN:OD1	2:H:59:ASN:HB2	2.18	0.43
3:I:27:VAL:O	3:I:124:VAL:HA	2.18	0.43
3:I:222:GLU:O	3:I:223:LYS:HD3	2.18	0.43
1:G:1670:VAL:HG22	1:G:1695:LEU:HD23	1.99	0.43
3:F:123:THR:HG23	5:F:406:HOH:O	2.18	0.43
3:C:35:LEU:N	3:C:35:LEU:HD12	2.33	0.43
2:H:99:ALA:HA	2:H:112:ILE:O	2.18	0.43
1:D:1463:GLY:O	1:D:1464:ALA:C	2.61	0.43
1:D:1683:ARG:NH1	1:D:1712:GLU:OE1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1697:SER:O	1:D:1724:ALA:HA	2.19	0.43
1:D:1885:ILE:HG22	1:D:1887:ILE:HG22	2.00	0.43
1:D:1489:ALA:CB	1:D:1618:VAL:HG11	2.49	0.43
1:D:1650:TRP:CH2	1:D:1885:ILE:HG21	2.54	0.43
1:A:1491:ARG:HA	1:A:1494:LEU:HB2	2.00	0.43
2:E:2:ALA:HA	2:E:102:PRO:HB3	2.01	0.43
2:E:49:TRP:CZ2	2:E:51:GLY:HA2	2.53	0.43
3:C:200:THR:O	3:C:203:GLN:HB2	2.19	0.43
1:D:1475:LEU:CD1	1:D:1525:VAL:HG21	2.47	0.43
2:E:125:SER:O	2:E:126:THR:HB	2.19	0.43
1:D:1447:MET:O	1:D:1449:GLU:N	2.50	0.43
1:G:1685:LEU:HD12	1:G:1685:LEU:HA	1.89	0.43
2:E:90:SER:HA	2:E:121:VAL:CG2	2.49	0.43
2:E:164:TRP:CD1	2:E:173:VAL:CG2	3.02	0.43
3:F:199:LEU:HD12	3:F:204:TRP:HB2	2.00	0.43
3:C:151:LEU:HB2	3:C:197:LEU:HB3	2.00	0.43
1:G:1662:TRP:HE1	1:G:1793:THR:HG22	1.83	0.43
2:E:160:VAL:HG13	2:E:208:VAL:CG1	2.49	0.43
2:E:174:HIS:O	2:E:176:PHE:CE1	2.71	0.43
3:I:143:GLU:O	3:I:148:LYS:CB	2.67	0.43
1:D:1688:ARG:CD	1:D:1874:GLN:HE22	2.32	0.43
1:D:1827:ARG:NH1	1:D:1833:PRO:O	2.51	0.43
1:G:1648:ARG:O	1:G:1906:LEU:HD23	2.19	0.42
2:B:38:TRP:CE2	2:B:83:MET:HB2	2.54	0.42
3:C:130:ALA:O	3:C:158:PHE:HA	2.19	0.42
3:C:160:PRO:HD2	3:C:216:HIS:CE1	2.54	0.42
3:C:160:PRO:HB3	3:C:217:GLU:OE2	2.19	0.42
1:D:1595:VAL:O	1:D:1598:VAL:HG22	2.18	0.42
1:G:1758:ASP:HB2	2:B:107:TYR:CZ	2.53	0.42
2:E:162:VAL:HA	2:E:207:ASN:O	2.19	0.42
1:A:1795:PHE:CE2	1:A:1797:LEU:HD21	2.53	0.42
2:E:61:ASN:ND2	3:F:112:ALA:HB3	2.34	0.42
3:I:51:TYR:HB2	3:I:106:LEU:HB3	2.01	0.42
3:I:144:LEU:HD12	3:I:148:LYS:CB	2.49	0.42
2:B:89:ARG:NH1	2:B:90:SER:OG	2.51	0.42
2:B:131:VAL:HG11	2:B:208:VAL:CG1	2.50	0.42
1:A:1603:ASN:C	1:A:1603:ASN:ND2	2.78	0.42
1:A:1603:ASN:C	1:A:1603:ASN:HD22	2.25	0.42
1:A:1611:VAL:HA	1:A:1638:LEU:O	2.18	0.42
2:E:164:TRP:HB3	2:E:169:LEU:HB3	2.01	0.42
3:F:163:VAL:CG2	3:F:214:VAL:HG13	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1824:ALA:HA	1:D:1834:ALA:HB1	2.01	0.42
1:G:1598:VAL:O	1:G:1598:VAL:CG2	2.66	0.42
1:G:1674:THR:HG21	1:G:1697:SER:OG	2.20	0.42
3:C:148:LYS:H	3:C:201:PRO:HG3	1.85	0.42
1:D:1464:ALA:HB1	1:D:1631:GLY:HA3	2.01	0.42
1:D:1593:TRP:HB3	1:D:1597:ARG:NH2	2.35	0.42
1:G:1483:ALA:O	1:G:1484:ASP:C	2.62	0.42
2:E:165:ASN:HA	2:E:205:ILE:HG12	2.01	0.42
3:F:168:LYS:HD3	3:F:213:GLN:NE2	2.35	0.42
2:B:90:SER:HA	2:B:121:VAL:CG2	2.49	0.42
2:H:30:THR:HG21	1:A:1763:THR:HG21	2.02	0.42
1:G:1589:HIS:O	1:G:1592:LEU:HB2	2.20	0.42
2:B:211:LYS:N	2:B:212:PRO:CD	2.83	0.42
2:H:53:ILE:CD1	2:H:73:THR:HA	2.50	0.42
1:D:1474:TRP:CH2	1:D:1629:VAL:CG1	3.03	0.42
2:E:111:ASP:HA	3:F:63:THR:HG21	2.02	0.42
1:D:1463:GLY:HA3	1:D:1645:VAL:HG21	2.02	0.42
1:G:1771:ARG:O	3:C:49:TYR:OH	2.33	0.41
1:D:1538:GLU:CG	1:D:1538:GLU:O	2.68	0.41
1:D:1910:ILE:HD12	1:D:1910:ILE:O	2.20	0.41
1:A:1477:ALA:HA	1:A:1504:LEU:O	2.19	0.41
1:G:1593:TRP:HB3	1:G:1597:ARG:NH2	2.34	0.41
3:C:155:ILE:HG21	3:C:214:VAL:HG11	2.02	0.41
2:H:29:GLY:HA3	2:H:103:ASN:OD1	2.20	0.41
1:G:1627:ALA:O	1:G:1631:GLY:N	2.45	0.41
1:G:1684:TRP:CD1	1:G:1870:CYS:HB3	2.55	0.41
1:G:1774:ARG:O	1:G:1778:LEU:N	2.52	0.41
2:E:125:SER:O	2:E:126:THR:CB	2.69	0.41
2:E:148:LEU:O	2:E:148:LEU:HG	2.20	0.41
3:C:127:GLN:HG2	3:C:159:TYR:CG	2.56	0.41
2:H:205:ILE:HG22	2:H:220:LYS:HA	2.02	0.41
1:D:1661:GLU:O	1:D:1663:LYS:N	2.46	0.41
1:A:1572:THR:CG2	1:A:1612:ASP:HA	2.50	0.41
1:A:1604:PRO:CB	1:A:1902:ARG:HD2	2.50	0.41
1:G:1824:ALA:HA	1:G:1834:ALA:HB1	2.01	0.41
2:E:145:THR:HA	2:E:194:VAL:O	2.20	0.41
3:C:83:LEU:HD12	3:C:83:LEU:HA	1.93	0.41
1:D:1774:ARG:O	1:D:1778:LEU:HB2	2.20	0.41
1:A:1537:ALA:O	1:A:1538:GLU:CB	2.69	0.41
3:C:226:ALA:HA	3:C:227:PRO:HD2	1.89	0.41
3:I:78:ARG:NH2	3:I:99:ASP:CG	2.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1476:VAL:HG13	1:A:1476:VAL:O	2.20	0.41
1:A:1864:MET:HE2	1:A:1869:ALA:HB2	2.02	0.41
1:G:1662:TRP:NE1	1:G:1793:THR:HG22	2.36	0.41
3:C:159:TYR:HB3	3:C:160:PRO:CD	2.42	0.41
2:H:53:ILE:HD13	2:H:73:THR:HA	2.02	0.41
1:D:1598:VAL:HG21	1:D:1811:GLY:HA2	2.02	0.41
3:I:64:LEU:O	3:I:65:ILE:HD13	2.21	0.41
1:D:1555:LEU:HD13	1:D:1568:LEU:HD11	2.02	0.41
1:D:1681:ILE:HG12	1:D:1798:PHE:HZ	1.86	0.41
3:F:66:TYR:CZ	3:F:70:ASN:HB3	2.56	0.41
2:B:129:PRO:HB3	2:B:155:TYR:HB3	2.02	0.41
3:C:54:GLN:OE1	3:C:62:ARG:NH2	2.50	0.41
1:G:1572:THR:OG1	1:G:1612:ASP:OD1	2.29	0.41
1:G:1597:ARG:O	1:G:1601:LEU:HD12	2.20	0.41
1:G:1598:VAL:HG11	1:G:1811:GLY:HA2	2.02	0.41
2:E:31:PHE:CD1	2:E:31:PHE:C	2.99	0.41
2:E:99:ALA:HA	2:E:112:ILE:O	2.21	0.41
2:H:42:ALA:O	2:H:43:PRO:C	2.63	0.41
3:I:106:LEU:HD11	3:I:114:TRP:HB3	2.03	0.41
1:A:1681:ILE:HD11	1:A:1798:PHE:CE2	2.55	0.41
2:E:156:PHE:H	2:E:157:PRO:HD2	1.86	0.41
3:F:146:ALA:C	3:F:148:LYS:N	2.79	0.41
1:D:1515:LEU:CD2	1:D:1558:ALA:CB	2.99	0.41
1:A:1572:THR:HG23	1:A:1612:ASP:HA	2.02	0.41
1:D:1542:ALA:HA	1:D:1543:PRO:HD3	1.94	0.40
2:E:164:TRP:CD1	2:E:173:VAL:CG1	3.05	0.40
3:I:188:ASN:OD1	3:I:188:ASN:C	2.64	0.40
1:A:1787:THR:HB	1:A:1792:LEU:HD11	2.03	0.40
1:G:1733:VAL:HG23	1:G:1786:LEU:HD13	2.02	0.40
3:F:37:CYS:HB3	3:F:88:ALA:HB3	2.03	0.40
1:D:1688:ARG:HG3	1:D:1874:GLN:HE22	1.85	0.40
1:G:1621:LEU:HD13	1:G:1621:LEU:HA	1.88	0.40
2:E:158:GLU:O	2:E:159:PRO:C	2.64	0.40
3:F:52:TRP:CD2	3:F:90:LEU:HB2	2.57	0.40
1:G:1662:TRP:NE1	1:G:1793:THR:CG2	2.84	0.40
1:G:1709:LEU:CD2	1:G:1713:LEU:HD21	2.52	0.40
2:E:14:LYS:O	2:E:121:VAL:HA	2.21	0.40
1:D:1691:PRO:HB2	1:D:1692:HIS:ND1	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	423/485 (87%)	376 (89%)	41 (10%)	6 (1%)	9	17
1	D	442/485 (91%)	402 (91%)	28 (6%)	12 (3%)	4	7
1	G	431/485 (89%)	380 (88%)	43 (10%)	8 (2%)	6	12
2	B	223/246 (91%)	200 (90%)	16 (7%)	7 (3%)	3	6
2	E	220/246 (89%)	181 (82%)	28 (13%)	11 (5%)	1	2
2	H	215/246 (87%)	193 (90%)	20 (9%)	2 (1%)	14	28
3	C	213/231 (92%)	186 (87%)	18 (8%)	9 (4%)	2	3
3	F	212/231 (92%)	183 (86%)	18 (8%)	11 (5%)	1	2
3	I	215/231 (93%)	185 (86%)	19 (9%)	11 (5%)	1	2
All	All	2594/2886 (90%)	2286 (88%)	231 (9%)	77 (3%)	3	6

All (77) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	1484	ASP
1	G	1539	PRO
1	G	1546	LEU
1	G	1615	ALA
2	E	125	SER
2	E	159	PRO
2	E	201	THR
2	E	221	VAL
3	F	171	SER
3	F	174	VAL
3	F	206	SER
2	B	140	SER
2	B	156	PHE
3	C	148	LYS
3	C	174	VAL
2	H	156	PHE

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Mol	Chain	Res	Type
3	I	146	ALA
3	I	147	ASN
3	I	159	TYR
1	D	1540	GLU
1	G	1449	GLU
2	E	126	THR
2	E	160	VAL
2	E	190	SER
3	F	187	SER
3	F	203	GLN
2	B	126	THR
3	C	177	GLY
3	I	85	GLY
3	I	149	ALA
3	I	170	ASP
3	I	176	ALA
1	D	1662	TRP
1	D	1892	ASP
1	A	1450	VAL
1	A	1537	ALA
1	A	1892	ASP
2	E	140	SER
3	F	98	GLU
3	F	150	THR
3	F	200	THR
3	C	145	GLN
3	C	149	ALA
3	I	144	LEU
1	D	1447	MET
1	D	1462	THR
1	A	1546	LEU
1	G	1577	ALA
2	E	94	ALA
2	B	142	SER
3	C	150	THR
3	C	172	SER
3	I	68	THR
3	I	125	LEU
1	D	1448	ASP
1	D	1585	ARG
1	G	1663	LYS
1	G	1677	VAL

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Mol	Chain	Res	Type
2	E	157	PRO
3	F	172	SER
2	B	67	GLN
2	B	77	SER
2	B	102	PRO
1	D	1666	GLY
1	D	1691	PRO
1	A	1538	GLU
1	A	1608	GLY
2	E	141	THR
3	F	16	GLN
3	F	159	TYR
2	H	107	TYR
1	D	1629	VAL
3	C	160	PRO
3	C	173	PRO
3	I	172	SER
1	D	1522	VAL
1	D	1466	GLU

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	295/348 (85%)	248 (84%)	47 (16%)	2	4
1	D	315/348 (90%)	276 (88%)	39 (12%)	4	8
1	G	314/348 (90%)	269 (86%)	45 (14%)	3	5
2	B	179/202 (89%)	152 (85%)	27 (15%)	3	4
2	E	182/202 (90%)	148 (81%)	34 (19%)	1	3
2	H	178/202 (88%)	156 (88%)	22 (12%)	4	8
3	C	170/191 (89%)	154 (91%)	16 (9%)	8	16
3	F	168/191 (88%)	145 (86%)	23 (14%)	3	6
3	I	172/191 (90%)	147 (86%)	25 (14%)	3	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1973/2223 (89%)	1695 (86%)	278 (14%)	3 6

All (278) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	1448	ASP
1	G	1450	VAL
1	G	1454	ARG
1	G	1460	ARG
1	G	1475	LEU
1	G	1505	VAL
1	G	1510	CYS
1	G	1521	SER
1	G	1524	GLU
1	G	1525	VAL
1	G	1560	VAL
1	G	1571	VAL
1	G	1592	LEU
1	G	1598	VAL
1	G	1613	VAL
1	G	1618	VAL
1	G	1621	LEU
1	G	1638	LEU
1	G	1645	VAL
1	G	1649	ARG
1	G	1651	VAL
1	G	1668	VAL
1	G	1670	VAL
1	G	1674	THR
1	G	1688	ARG
1	G	1698	ARG
1	G	1704	ASP
1	G	1708	GLU
1	G	1713	LEU
1	G	1720	THR
1	G	1735	GLU
1	G	1742	ASP
1	G	1743	ASP
1	G	1749	VAL
1	G	1774	ARG
1	G	1791	ASP
1	G	1827	ARG

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Mol	Chain	Res	Type
1	G	1828	ARG
1	G	1835	THR
1	G	1862	ILE
1	G	1867	GLU
1	G	1889	VAL
1	G	1896	LEU
1	G	1902	ARG
1	G	1906	LEU
2	E	3	GLU
2	E	4	VAL
2	E	7	VAL
2	E	13	VAL
2	E	31	PHE
2	E	33	SER
2	E	37	SER
2	E	39	VAL
2	E	59	ASN
2	E	60	THR
2	E	71	THR
2	E	74	THR
2	E	80	THR
2	E	83	MET
2	E	89	ARG
2	E	90	SER
2	E	93	THR
2	E	112	ILE
2	E	121	VAL
2	E	122	SER
2	E	138	SER
2	E	148	LEU
2	E	150	CYS
2	E	152	VAL
2	E	159	PRO
2	E	162	VAL
2	E	180	LEU
2	E	182	SER
2	E	203	THR
2	E	215	THR
2	E	217	VAL
2	E	219	LYS
2	E	220	LYS
2	E	224	LYS

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Mol	Chain	Res	Type
3	F	20	ILE
3	F	32	THR
3	F	41	THR
3	F	44	VAL
3	F	63	THR
3	F	73	SER
3	F	80	SER
3	F	93	SER
3	F	141	SER
3	F	144	LEU
3	F	151	LEU
3	F	152	VAL
3	F	160	PRO
3	F	165	VAL
3	F	170	ASP
3	F	175	LYS
3	F	179	GLU
3	F	181	THR
3	F	184	SER
3	F	203	GLN
3	F	204	TRP
3	F	206	SER
3	F	219	SER
2	B	9	SER
2	B	37	SER
2	B	39	VAL
2	B	40	ARG
2	B	71	THR
2	B	76	THR
2	B	79	SER
2	B	80	THR
2	B	89	ARG
2	B	121	VAL
2	B	130	SER
2	B	131	VAL
2	B	138	SER
2	B	160	VAL
2	B	161	THR
2	B	166	SER
2	B	171	SER
2	B	175	THR
2	B	188	LEU

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Mol	Chain	Res	Type
2	B	193	THR
2	B	196	SER
2	B	207	ASN
2	B	208	VAL
2	B	215	THR
2	B	217	VAL
2	B	219	LYS
2	B	221	VAL
3	C	32	THR
3	C	34	THR
3	C	39	SER
3	C	41	THR
3	C	63	THR
3	C	83	LEU
3	C	142	GLU
3	C	150	THR
3	C	156	SER
3	C	164	THR
3	C	170	ASP
3	C	175	LYS
3	C	181	THR
3	C	184	SER
3	C	194	SER
3	C	215	THR
2	H	13	VAL
2	H	32	SER
2	H	36	ILE
2	H	74	THR
2	H	79	SER
2	H	80	THR
2	H	93	THR
2	H	106	ASP
2	H	118	THR
2	H	121	VAL
2	H	123	SER
2	H	125	SER
2	H	127	LYS
2	H	138	SER
2	H	145	THR
2	H	160	VAL
2	H	182	SER
2	H	188	LEU

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Mol	Chain	Res	Type
2	H	189	SER
2	H	198	SER
2	H	206	CYS
2	H	215	THR
3	I	16	GLN
3	I	19	VAL
3	I	26	THR
3	I	32	THR
3	I	34	THR
3	I	41	THR
3	I	68	THR
3	I	70	ASN
3	I	73	SER
3	I	80	SER
3	I	144	LEU
3	I	145	GLN
3	I	150	THR
3	I	163	VAL
3	I	175	LYS
3	I	178	VAL
3	I	181	THR
3	I	182	THR
3	I	186[A]	GLN
3	I	186[B]	GLN
3	I	194	SER
3	I	198	SER
3	I	199	LEU
3	I	202	GLU
3	I	215	THR
1	D	1446	HIS
1	D	1448	ASP
1	D	1482	THR
1	D	1494	LEU
1	D	1505	VAL
1	D	1515	LEU
1	D	1518	ARG
1	D	1525	VAL
1	D	1528	VAL
1	D	1538	GLU
1	D	1540	GLU
1	D	1561	SER
1	D	1570	THR

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Mol	Chain	Res	Type
1	D	1597	ARG
1	D	1613	VAL
1	D	1620	GLU
1	D	1638	LEU
1	D	1645	VAL
1	D	1665	THR
1	D	1670	VAL
1	D	1685	LEU
1	D	1688	ARG
1	D	1698	ARG
1	D	1719	ARG
1	D	1720	THR
1	D	1722	VAL
1	D	1732	SER
1	D	1733	VAL
1	D	1742	ASP
1	D	1749	VAL
1	D	1762	ASP
1	D	1764	LEU
1	D	1769	ILE
1	D	1770	GLU
1	D	1790	LEU
1	D	1835	THR
1	D	1842	TRP
1	D	1881	GLU
1	D	1889	VAL
1	A	1449	GLU
1	A	1462	THR
1	A	1488	THR
1	A	1491	ARG
1	A	1510	CYS
1	A	1522	VAL
1	A	1525	VAL
1	A	1528	VAL
1	A	1531	LEU
1	A	1535	ASP
1	A	1546	LEU
1	A	1548	SER
1	A	1554	SER
1	A	1583	ARG
1	A	1625	LEU
1	A	1635	GLU

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Mol	Chain	Res	Type
1	A	1645	VAL
1	A	1665	THR
1	A	1668	VAL
1	A	1669	LEU
1	A	1677	VAL
1	A	1694	LEU
1	A	1704	ASP
1	A	1713	LEU
1	A	1719	ARG
1	A	1720	THR
1	A	1722	VAL
1	A	1731	GLU
1	A	1733	VAL
1	A	1734	ARG
1	A	1747	SER
1	A	1756	LEU
1	A	1760	THR
1	A	1786	LEU
1	A	1789	GLU
1	A	1790	LEU
1	A	1791	ASP
1	A	1800	SER
1	A	1855	ARG
1	A	1857	ARG
1	A	1881	GLU
1	A	1893	ARG
1	A	1895	LEU
1	A	1896	LEU
1	A	1899	THR
1	A	1902	ARG
1	A	1904	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	1589	HIS
1	G	1784	HIS
1	G	1826	GLN
2	E	61	ASN
2	E	67	GLN
2	E	202	GLN
3	F	213	GLN

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Mol	Chain	Res	Type
2	B	59	ASN
2	B	174	HIS
2	B	181	GLN
3	C	70	ASN
3	C	186	GLN
2	H	174	HIS
1	D	1586	ASN
1	D	1825	GLN
1	D	1874	GLN
1	D	1875	ASN
1	A	1557	GLN
1	A	1603	ASN
1	A	1874	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

7 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	SO4	D	2001	-	4,4,4	0.34	0	6,6,6	0.06	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	SO4	E	301	-	4,4,4	0.33	0	6,6,6	0.12	0
4	SO4	A	2001	-	4,4,4	0.36	0	6,6,6	0.06	0
4	SO4	C	301	-	4,4,4	0.34	0	6,6,6	0.05	0
4	SO4	F	301	-	4,4,4	0.33	0	6,6,6	0.08	0
4	SO4	G	2001	-	4,4,4	0.35	0	6,6,6	0.08	0
4	SO4	B	301	-	4,4,4	0.31	0	6,6,6	0.08	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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, 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	431/485 (88%)	0.53	22 (5%) 33 33	89, 144, 181, 212	0
1	D	450/485 (92%)	0.36	13 (2%) 53 52	76, 121, 160, 211	0
1	G	439/485 (90%)	0.34	13 (2%) 52 50	76, 119, 164, 209	0
2	B	225/246 (91%)	-0.12	2 (0%) 81 81	61, 86, 111, 162	0
2	E	224/246 (91%)	0.72	35 (15%) 5 4	75, 104, 159, 232	0
2	H	219/246 (89%)	-0.04	2 (0%) 81 81	57, 83, 109, 149	0
3	C	215/231 (93%)	-0.23	8 (3%) 45 42	55, 69, 101, 152	0
3	F	216/231 (93%)	0.02	8 (3%) 45 42	57, 76, 111, 153	0
3	I	216/231 (93%)	-0.10	5 (2%) 61 59	34, 75, 113, 142	1 (0%)
All	All	2635/2886 (91%)	0.23	108 (4%) 41 39	34, 104, 164, 232	1 (0%)

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	205	ILE	7.6
3	F	201	PRO	6.5
1	G	1910	ILE	5.7
2	E	206	CYS	5.3
3	F	200	THR	5.1
2	E	157	PRO	4.6
2	E	203	THR	4.3
1	A	1653	ALA	4.1
1	G	1842	TRP	4.0
3	F	202	GLU	4.0
2	E	156	PHE	4.0
2	B	2	ALA	4.0
1	D	1662	TRP	3.8
1	A	1875	ASN	3.7
2	E	164	TRP	3.7

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Mol	Chain	Res	Type	RSRZ
2	E	213	SER	3.7
1	A	1856	PHE	3.7
1	G	1844	GLY	3.7
2	E	174	HIS	3.6
1	G	1463	GLY	3.6
1	D	1843	ALA	3.6
1	G	1655	ALA	3.4
3	I	174	VAL	3.4
1	D	1655	ALA	3.4
3	F	149	ALA	3.4
3	C	160	PRO	3.4
2	E	221	VAL	3.4
3	I	147	ASN	3.3
2	H	124	ALA	3.3
3	I	146	ALA	3.2
2	E	159	PRO	3.1
1	G	1684	TRP	3.1
1	A	1628	VAL	3.1
3	F	160	PRO	3.1
2	E	135	ALA	3.1
1	G	1856	PHE	3.0
2	E	167	GLY	3.0
3	C	148	LYS	3.0
3	I	186[A]	GLN	3.0
1	D	1654	ALA	2.9
3	C	174	VAL	2.9
1	G	1870	CYS	2.9
1	A	1907	PHE	2.9
1	A	1474	TRP	2.9
1	A	1627	ALA	2.9
2	E	192	VAL	2.8
1	D	1910	ILE	2.8
2	E	136	PRO	2.8
2	E	166	SER	2.8
1	A	1497	ALA	2.8
3	C	146	ALA	2.8
2	E	150	CYS	2.7
2	E	210	HIS	2.7
1	D	1622	ALA	2.7
2	H	32	SER	2.7
2	E	132	PHE	2.7
2	E	172	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	1898	TYR	2.6
2	E	158	GLU	2.6
1	G	1508	ALA	2.6
1	A	1892	ASP	2.6
2	B	143	GLY	2.6
3	C	159	TYR	2.6
1	A	1673	GLY	2.6
2	E	130	SER	2.5
1	A	1522	VAL	2.5
1	D	1805	PHE	2.5
1	A	1664	PRO	2.4
3	F	144	LEU	2.4
1	A	1478	LYS	2.4
3	F	175	LYS	2.4
1	A	1650	TRP	2.4
2	E	215	THR	2.3
3	F	150	THR	2.3
1	G	1762	ASP	2.3
2	E	202	GLN	2.3
1	A	1476	VAL	2.3
1	A	1602	GLU	2.3
3	C	145	GLN	2.3
1	A	1684	TRP	2.3
1	D	1853	ALA	2.3
2	E	191	VAL	2.3
3	C	16	GLN	2.2
1	D	1885	ILE	2.2
1	D	1467	PRO	2.2
1	D	1659	ASP	2.2
2	E	194	VAL	2.2
3	C	176	ALA	2.2
2	E	190	SER	2.2
2	E	217	VAL	2.2
1	A	1533	ALA	2.2
1	A	1855	ARG	2.2
1	D	1626	ALA	2.1
2	E	207	ASN	2.1
2	E	38	TRP	2.1
2	E	162	VAL	2.1
2	E	189	SER	2.1
1	A	1639	ALA	2.1
2	E	208	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	1477	ALA	2.0
3	I	175	LYS	2.0
2	E	148	LEU	2.0
2	E	160	VAL	2.0
1	A	1572	THR	2.0
1	G	1859	HIS	2.0
1	G	1673	GLY	2.0
2	E	36	ILE	2.0
1	G	1861	VAL	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
4	SO4	E	301	5/5	0.75	0.08	118,123,130,136	0
4	SO4	F	301	5/5	0.76	0.08	123,128,132,135	0
4	SO4	B	301	5/5	0.83	0.08	109,116,127,128	0
4	SO4	C	301	5/5	0.88	0.07	127,129,132,132	0
4	SO4	G	2001	5/5	0.90	0.09	86,89,101,104	0
4	SO4	A	2001	5/5	0.94	0.08	88,94,101,105	0
4	SO4	D	2001	5/5	0.95	0.06	87,90,96,96	0

6.5 Other polymers [i](#)

There are no such residues in this entry.