



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:45 AM UTC

PDB ID : 7OX5 / pdb_00007ox5
Title : hIL-9:hIL-9Ra complex
Authors : De Vos, T.; Savvides, S.N.
Deposited on : 2021-06-22
Resolution : 3.09 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

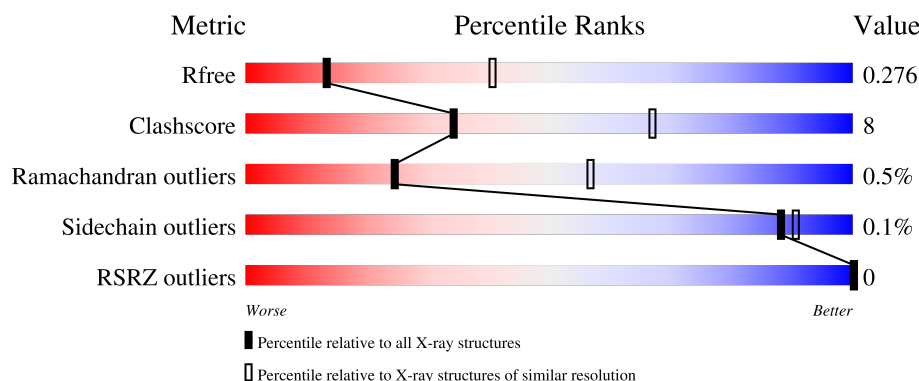
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

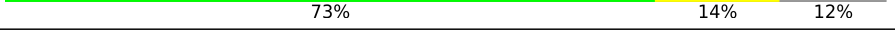
The reported resolution of this entry is 3.09 Å.

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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	226	
1	C	226	
1	E	226	
1	G	226	
1	I	226	

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Mol	Chain	Length	Quality of chain
1	K	226	
1	M	226	
1	O	226	
2	B	130	
2	D	130	
2	F	130	
2	H	130	
2	J	130	
2	L	130	
2	N	130	
2	P	130	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	A	301	-	-	X	-
3	SO4	B	201	-	-	X	-
3	SO4	D	201	-	-	X	-
3	SO4	G	301	-	-	X	-
3	SO4	J	201	-	-	X	-
3	SO4	O	301	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 39121 atoms, of which 19307 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 Interleukin-9 receptor.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	208	Total	C	H	N	O	S	0	0	0
			3247	1049	1589	287	312	10			
1	C	206	Total	C	H	N	O	S	0	0	0
			3221	1043	1577	281	310	10			
1	E	176	Total	C	H	N	O	S	0	0	0
			2802	912	1378	244	260	8			
1	G	198	Total	C	H	N	O	S	0	0	0
			3118	1011	1526	272	299	10			
1	I	182	Total	C	H	N	O	S	0	0	0
			2888	941	1416	250	272	9			
1	K	188	Total	C	H	N	O	S	0	0	0
			2940	960	1442	253	275	10			
1	M	199	Total	C	H	N	O	S	0	0	0
			3133	1018	1532	273	301	9			
1	O	188	Total	C	H	N	O	S	0	0	0
			2955	958	1450	261	277	9			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	36	GLY	-	expression tag	UNP Q01113
A	37	SER	-	expression tag	UNP Q01113
A	38	HIS	-	expression tag	UNP Q01113
A	39	MET	-	expression tag	UNP Q01113
C	36	GLY	-	expression tag	UNP Q01113
C	37	SER	-	expression tag	UNP Q01113
C	38	HIS	-	expression tag	UNP Q01113
C	39	MET	-	expression tag	UNP Q01113
E	36	GLY	-	expression tag	UNP Q01113
E	37	SER	-	expression tag	UNP Q01113
E	38	HIS	-	expression tag	UNP Q01113
E	39	MET	-	expression tag	UNP Q01113
G	36	GLY	-	expression tag	UNP Q01113

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Chain	Residue	Modelled	Actual	Comment	Reference
G	37	SER	-	expression tag	UNP Q01113
G	38	HIS	-	expression tag	UNP Q01113
G	39	MET	-	expression tag	UNP Q01113
I	36	GLY	-	expression tag	UNP Q01113
I	37	SER	-	expression tag	UNP Q01113
I	38	HIS	-	expression tag	UNP Q01113
I	39	MET	-	expression tag	UNP Q01113
K	36	GLY	-	expression tag	UNP Q01113
K	37	SER	-	expression tag	UNP Q01113
K	38	HIS	-	expression tag	UNP Q01113
K	39	MET	-	expression tag	UNP Q01113
M	36	GLY	-	expression tag	UNP Q01113
M	37	SER	-	expression tag	UNP Q01113
M	38	HIS	-	expression tag	UNP Q01113
M	39	MET	-	expression tag	UNP Q01113
O	36	GLY	-	expression tag	UNP Q01113
O	37	SER	-	expression tag	UNP Q01113
O	38	HIS	-	expression tag	UNP Q01113
O	39	MET	-	expression tag	UNP Q01113

- Molecule 2 is a protein called Interleukin-9.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	119	Total	C	H	N	O	S	0	0	0
			1850	576	926	160	174	14			
2	D	116	Total	C	H	N	O	S	0	0	0
			1814	565	913	156	166	14			
2	F	119	Total	C	H	N	O	S	0	0	0
			1850	576	926	160	174	14			
2	H	119	Total	C	H	N	O	S	0	0	0
			1850	576	926	160	174	14			
2	J	119	Total	C	H	N	O	S	0	0	0
			1850	576	926	160	174	14			
2	L	121	Total	C	H	N	O	S	0	0	0
			1874	583	938	162	176	15			
2	N	119	Total	C	H	N	O	S	0	0	0
			1850	576	926	160	174	14			
2	P	117	Total	C	H	N	O	S	0	0	0
			1823	567	916	156	170	14			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	15	GLY	-	expression tag	UNP P15248
B	16	SER	-	expression tag	UNP P15248
B	17	HIS	-	expression tag	UNP P15248
B	18	MET	-	expression tag	UNP P15248
D	15	GLY	-	expression tag	UNP P15248
D	16	SER	-	expression tag	UNP P15248
D	17	HIS	-	expression tag	UNP P15248
D	18	MET	-	expression tag	UNP P15248
F	15	GLY	-	expression tag	UNP P15248
F	16	SER	-	expression tag	UNP P15248
F	17	HIS	-	expression tag	UNP P15248
F	18	MET	-	expression tag	UNP P15248
H	15	GLY	-	expression tag	UNP P15248
H	16	SER	-	expression tag	UNP P15248
H	17	HIS	-	expression tag	UNP P15248
H	18	MET	-	expression tag	UNP P15248
J	15	GLY	-	expression tag	UNP P15248
J	16	SER	-	expression tag	UNP P15248
J	17	HIS	-	expression tag	UNP P15248
J	18	MET	-	expression tag	UNP P15248
L	15	GLY	-	expression tag	UNP P15248
L	16	SER	-	expression tag	UNP P15248
L	17	HIS	-	expression tag	UNP P15248
L	18	MET	-	expression tag	UNP P15248
N	15	GLY	-	expression tag	UNP P15248
N	16	SER	-	expression tag	UNP P15248
N	17	HIS	-	expression tag	UNP P15248
N	18	MET	-	expression tag	UNP P15248
P	15	GLY	-	expression tag	UNP P15248
P	16	SER	-	expression tag	UNP P15248
P	17	HIS	-	expression tag	UNP P15248
P	18	MET	-	expression tag	UNP P15248

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	I	1	Total	O	S	0	0
			5	4	1		
3	J	1	Total	O	S	0	0
			5	4	1		
3	N	1	Total	O	S	0	0
			5	4	1		
3	O	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

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

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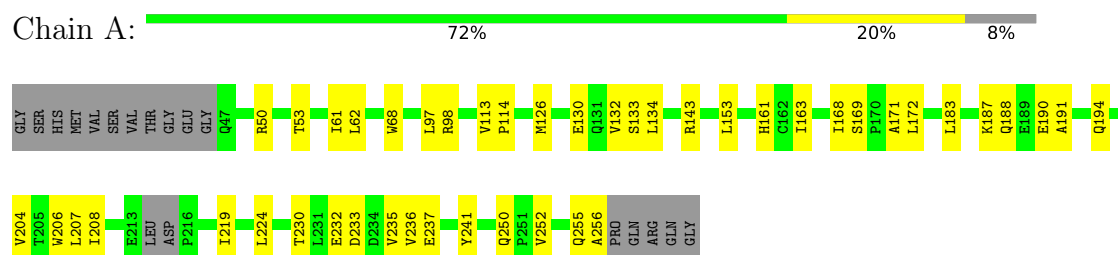
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	K	1	Total 1	O 1	0	0
4	O	1	Total 1	O 1	0	0
4	P	1	Total 1	O 1	0	0

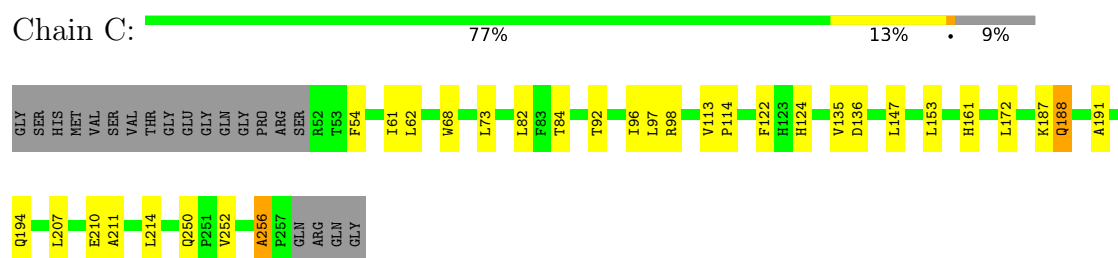
3 Residue-property plots [i](#)

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.

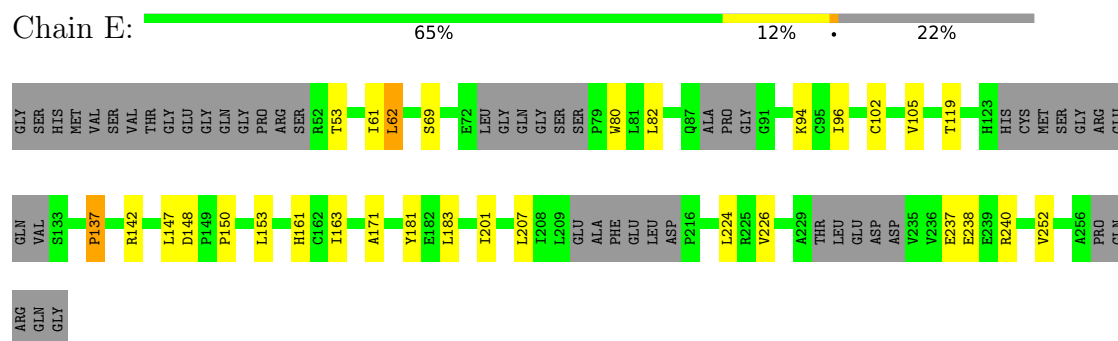
• Molecule 1: Interleukin-9 receptor



• Molecule 1: Interleukin-9 receptor

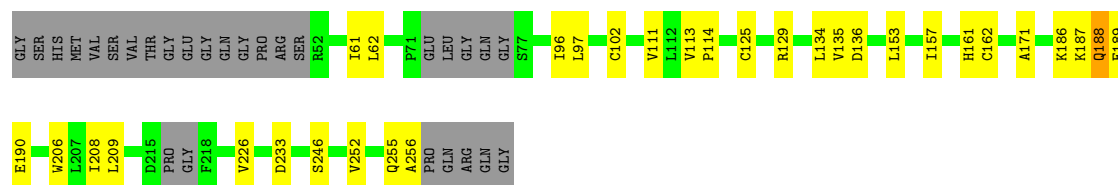


• Molecule 1: Interleukin-9 receptor

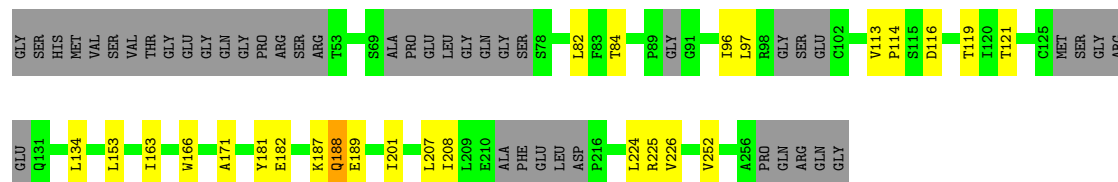


• Molecule 1: Interleukin-9 receptor

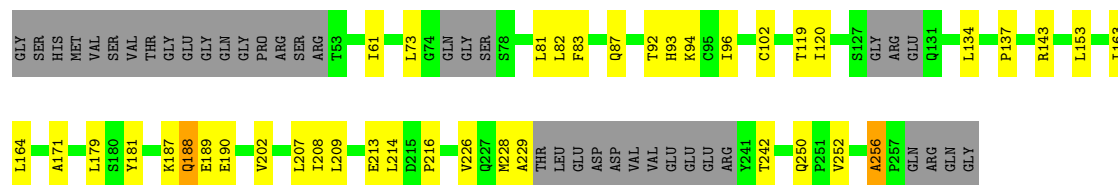




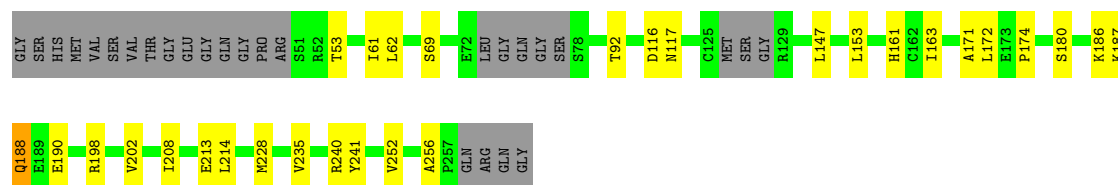
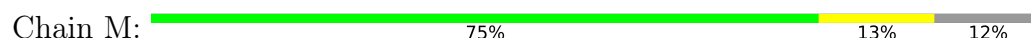
- Molecule 1: Interleukin-9 receptor



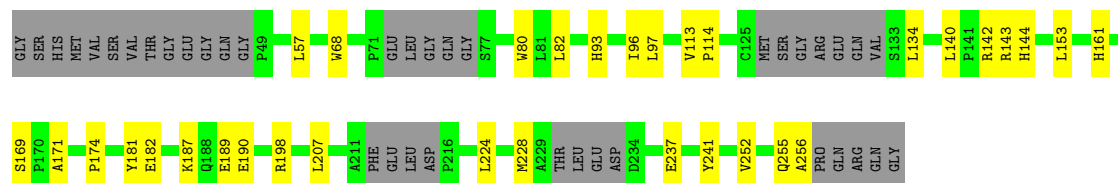
- Molecule 1: Interleukin-9 receptor



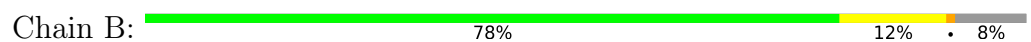
- Molecule 1: Interleukin-9 receptor

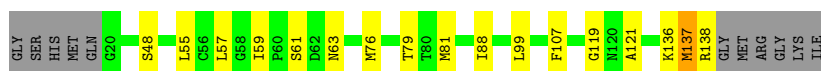


- Molecule 1: Interleukin-9 receptor

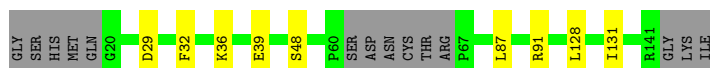
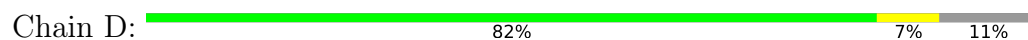


- Molecule 2: Interleukin-9

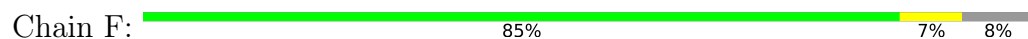




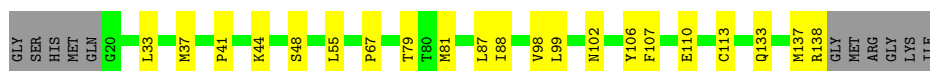
• Molecule 2: Interleukin-9



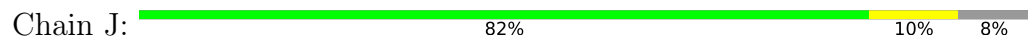
• Molecule 2: Interleukin-9



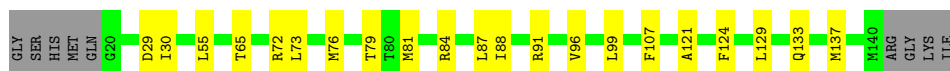
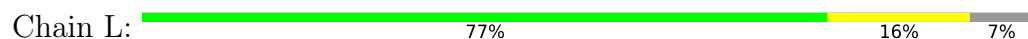
• Molecule 2: Interleukin-9



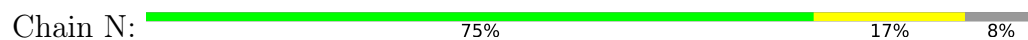
• Molecule 2: Interleukin-9



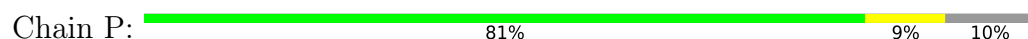
• Molecule 2: Interleukin-9



• Molecule 2: Interleukin-9



• Molecule 2: Interleukin-9



GLY	SER	HIS	MET	GLN	G20	M63	C64	T65	R66	M81	I88	R91	L99	Y106	F107	G113	ASN	GLN	T116	A121	K134	R138	GLY	MET	ARG	GLY	LYS	ILE
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.45Å 107.81Å 159.55Å 90.00° 90.77° 90.00°	Depositor
Resolution (Å)	47.69 – 3.09 47.69 – 3.09	Depositor EDS
% Data completeness (in resolution range)	98.8 (47.69-3.09) 98.9 (47.69-3.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 3.07Å)	Xtriage
Refinement program	PHENIX 1.19.1	Depositor
R, R_{free}	0.220 , 0.280 0.218 , 0.276	Depositor DCC
R_{free} test set	2641 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	111.4	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 96.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.079 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	39121	wwPDB-VP
Average B, all atoms (Å ²)	135.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.11% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.13	0/1705	0.39	0/2325
1	C	0.12	0/1692	0.36	0/2312
1	E	0.10	0/1463	0.29	0/1992
1	G	0.12	0/1636	0.37	0/2232
1	I	0.11	0/1512	0.33	0/2062
1	K	0.11	0/1543	0.34	0/2108
1	M	0.12	0/1647	0.37	0/2250
1	O	0.12	0/1548	0.38	0/2110
2	B	0.17	0/939	0.46	0/1266
2	D	0.16	0/915	0.52	0/1229
2	F	0.15	0/939	0.43	0/1266
2	H	0.18	0/939	0.57	0/1266
2	J	0.14	0/939	0.45	0/1266
2	L	0.14	0/951	0.50	0/1281
2	N	0.14	0/939	0.48	0/1266
2	P	0.14	0/921	0.44	0/1240
All	All	0.13	0/20228	0.41	0/27471

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	1658	1589	1589	38	0
1	C	1644	1577	1575	24	0
1	E	1424	1378	1377	27	0
1	G	1592	1526	1525	32	0
1	I	1472	1416	1415	22	0
1	K	1498	1442	1440	31	0
1	M	1601	1532	1531	27	0
1	O	1505	1450	1449	34	0
2	B	924	926	926	12	0
2	D	901	913	913	9	0
2	F	924	926	926	5	0
2	H	924	926	926	16	0
2	J	924	926	926	10	1
2	L	936	938	938	16	1
2	N	924	926	926	15	0
2	P	907	916	915	11	0
3	A	5	0	0	2	0
3	B	5	0	0	2	0
3	D	5	0	0	2	0
3	F	5	0	0	0	0
3	G	5	0	0	4	0
3	H	5	0	0	1	0
3	I	5	0	0	0	0
3	J	5	0	0	2	0
3	N	5	0	0	0	0
3	O	5	0	0	5	0
4	B	2	0	0	0	0
4	H	1	0	0	0	0
4	K	1	0	0	0	0
4	O	1	0	0	1	0
4	P	1	0	0	0	0
All	All	19814	19307	19297	298	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (298) 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:E:163:ILE:HD12	1:G:206:TRP:CZ3	1.97	1.00
1:O:143:ARG:NH1	1:O:237:GLU:OE2	1.96	0.97
1:A:163:ILE:HD12	1:A:208:ILE:HG22	1.52	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:48:SER:OG	3:D:201:SO4:O1	1.99	0.80
1:M:235:VAL:O	1:M:240:ARG:NH1	2.15	0.79
1:G:125:CYS:SG	1:G:129:ARG:NH1	2.56	0.79
2:B:48:SER:OG	3:B:201:SO4:O2	2.00	0.78
1:G:171:ALA:HB2	2:H:87:LEU:HD23	1.63	0.78
1:I:181:TYR:HD2	1:I:224:LEU:HD21	1.49	0.76
1:A:143:ARG:NH1	1:A:237:GLU:OE2	2.19	0.75
2:L:99:LEU:HD13	2:L:107:PHE:CE2	2.23	0.73
1:E:183:LEU:HD22	1:E:207:LEU:HD11	1.71	0.72
1:E:150:PRO:HG2	1:E:224:LEU:CD1	2.21	0.71
1:E:142:ARG:NH2	1:E:237:GLU:O	2.23	0.70
1:A:163:ILE:CD1	1:A:208:ILE:HG22	2.22	0.69
1:I:187:LYS:O	1:I:189:GLU:N	2.25	0.69
1:K:73:LEU:HD12	1:K:73:LEU:O	1.93	0.69
2:J:48:SER:OG	3:J:201:SO4:O4	2.12	0.68
2:P:106:TYR:OH	2:P:134:LYS:NZ	2.26	0.68
1:M:163:ILE:HD12	1:M:208:ILE:HG22	1.74	0.68
1:O:228:MET:HE2	1:O:241:TYR:CD2	2.29	0.68
1:M:153:LEU:O	1:M:252:VAL:HG11	1.94	0.68
2:J:48:SER:OG	3:J:201:SO4:S	2.51	0.67
1:K:187:LYS:O	1:K:190:GLU:N	2.25	0.67
2:L:76:MET:HE1	2:L:124:PHE:CE2	2.30	0.67
1:M:161:HIS:NE2	3:O:301:SO4:S	2.62	0.66
1:E:161:HIS:NE2	3:G:301:SO4:O4	2.28	0.66
1:E:150:PRO:HG2	1:E:224:LEU:HD12	1.78	0.66
1:A:204:VAL:HG22	1:A:206:TRP:H	1.62	0.65
1:K:187:LYS:O	1:K:189:GLU:N	2.29	0.65
1:A:183:LEU:HD22	1:A:207:LEU:HD11	1.79	0.64
1:G:161:HIS:NE2	3:G:301:SO4:O1	2.29	0.64
1:I:182:GLU:OE2	1:I:225:ARG:NH2	2.30	0.64
1:O:142:ARG:NH2	1:O:237:GLU:OE2	2.30	0.64
1:A:68:TRP:CE3	1:A:97:LEU:HD23	2.33	0.64
1:G:187:LYS:O	1:G:189:GLU:N	2.31	0.63
2:H:99:LEU:HD13	2:H:107:PHE:CE2	2.34	0.62
1:A:187:LYS:O	1:A:190:GLU:N	2.32	0.62
1:C:73:LEU:HD13	1:C:124:HIS:ND1	2.15	0.62
2:B:48:SER:OG	3:B:201:SO4:S	2.57	0.62
2:L:55:LEU:HD23	2:L:79:THR:HG22	1.82	0.62
1:E:161:HIS:NE2	3:G:301:SO4:S	2.71	0.62
1:O:161:HIS:NE2	3:O:301:SO4:O2	2.32	0.62
1:C:82:LEU:CD2	1:C:84:THR:HG23	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:209:LEU:HD22	1:K:213:GLU:OE2	2.00	0.61
1:O:161:HIS:NE2	3:O:301:SO4:S	2.72	0.61
1:O:181:TYR:HB3	1:O:224:LEU:HD11	1.81	0.61
1:A:232:GLU:N	1:A:232:GLU:OE1	2.33	0.61
1:E:163:ILE:HD11	1:G:208:ILE:HD11	1.82	0.61
1:O:97:LEU:HD23	1:O:97:LEU:H	1.65	0.61
2:P:65:THR:HG23	2:P:66:ARG:HG2	1.82	0.60
1:K:153:LEU:HD23	1:K:153:LEU:H	1.67	0.60
1:A:208:ILE:O	1:A:208:ILE:HD12	2.01	0.60
1:A:153:LEU:O	1:A:252:VAL:HG11	2.02	0.60
1:I:97:LEU:H	1:I:97:LEU:HD23	1.66	0.60
2:J:55:LEU:HD23	2:J:79:THR:HG22	1.84	0.59
1:O:171:ALA:O	2:P:91:ARG:NH2	2.33	0.59
1:O:198:ARG:NH2	4:O:401:HOH:O	2.33	0.59
1:A:153:LEU:HD23	1:A:153:LEU:H	1.68	0.59
1:G:153:LEU:H	1:G:153:LEU:HD23	1.67	0.58
1:K:143:ARG:O	1:K:242:THR:OG1	2.21	0.58
2:F:81:MET:HE1	2:F:121:ALA:HB1	1.85	0.58
1:A:230:THR:HG22	1:A:241:TYR:O	2.04	0.58
1:G:161:HIS:NE2	3:G:301:SO4:S	2.76	0.58
1:C:68:TRP:CE3	1:C:97:LEU:HD23	2.38	0.58
1:A:169:SER:HA	2:D:39:GLU:OE2	2.03	0.58
1:M:163:ILE:CD1	1:M:208:ILE:HG22	2.33	0.58
1:C:98:ARG:NH1	2:H:110:GLU:OE2	2.37	0.58
1:K:171:ALA:HB2	2:L:87:LEU:HD23	1.85	0.58
1:I:153:LEU:HD23	1:I:153:LEU:H	1.68	0.57
2:B:55:LEU:HD23	2:B:79:THR:HG22	1.86	0.57
2:N:81:MET:HE1	2:N:121:ALA:HB1	1.86	0.57
1:E:163:ILE:HD12	1:G:206:TRP:CE3	2.38	0.57
1:M:161:HIS:NE2	3:O:301:SO4:O1	2.37	0.57
3:A:301:SO4:O1	1:C:161:HIS:NE2	2.38	0.56
1:C:210:GLU:O	1:C:211:ALA:HB3	2.04	0.56
1:C:153:LEU:HD23	1:C:153:LEU:H	1.69	0.56
1:K:171:ALA:HA	2:L:88:ILE:HD11	1.86	0.56
1:E:150:PRO:HG2	1:E:224:LEU:HD11	1.87	0.56
1:O:153:LEU:HD23	1:O:153:LEU:H	1.70	0.56
2:J:137:MET:O	2:J:138:ARG:HB2	2.05	0.56
1:K:82:LEU:HD12	1:K:93:HIS:O	2.06	0.56
2:B:81:MET:HE1	2:B:121:ALA:HB1	1.87	0.56
2:L:29:ASP:OD2	2:L:91:ARG:HD2	2.05	0.55
1:E:163:ILE:HD12	1:G:206:TRP:CH2	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:153:LEU:HD23	1:M:153:LEU:H	1.72	0.55
1:E:82:LEU:HD12	1:E:94:LYS:HB3	1.88	0.55
1:K:187:LYS:O	1:K:188:GLN:C	2.50	0.55
1:A:169:SER:HB2	1:A:172:LEU:HD23	1.90	0.54
1:O:57:LEU:HD13	1:O:144:HIS:HB3	1.89	0.54
1:I:171:ALA:HA	2:J:88:ILE:HD11	1.89	0.54
1:C:153:LEU:HD21	1:C:250:GLN:O	2.07	0.54
1:G:171:ALA:HA	2:H:88:ILE:HD11	1.89	0.54
2:L:81:MET:HE1	2:L:121:ALA:HB1	1.89	0.54
2:H:55:LEU:HD23	2:H:79:THR:HG22	1.88	0.54
1:I:187:LYS:O	1:I:188:GLN:C	2.51	0.54
2:L:65:THR:HG22	2:L:65:THR:O	2.08	0.54
1:M:161:HIS:NE2	3:O:301:SO4:O3	2.41	0.54
2:J:29:ASP:OD2	2:J:91:ARG:HD2	2.07	0.54
2:D:48:SER:OG	3:D:201:SO4:S	2.66	0.53
2:F:99:LEU:HD13	2:F:107:PHE:CZ	2.44	0.53
2:N:64:CYS:SG	2:N:65:THR:N	2.81	0.53
2:N:39:GLU:OE2	1:O:169:SER:HA	2.08	0.53
1:M:147:LEU:HD22	1:M:172:LEU:HD21	1.91	0.53
1:I:113:VAL:HG12	1:I:116:ASP:OD1	2.08	0.53
1:O:68:TRP:CE3	1:O:97:LEU:HD12	2.43	0.53
1:I:187:LYS:O	1:I:187:LYS:CG	2.57	0.53
1:A:134:LEU:N	1:A:134:LEU:HD22	2.24	0.53
1:K:153:LEU:O	1:K:252:VAL:HG11	2.08	0.53
1:G:187:LYS:HD3	1:G:190:GLU:HG3	1.90	0.52
1:O:174:PRO:HG2	2:P:88:ILE:HD12	1.90	0.52
1:C:187:LYS:O	1:C:188:GLN:C	2.51	0.52
2:J:99:LEU:HD13	2:J:107:PHE:CZ	2.44	0.52
1:G:96:ILE:HD12	1:G:96:ILE:H	1.73	0.52
1:G:226:VAL:O	1:G:246:SER:OG	2.24	0.52
1:K:228:MET:O	1:K:229:ALA:HB2	2.10	0.52
2:J:99:LEU:HD13	2:J:107:PHE:CE2	2.45	0.52
1:I:163:ILE:CD1	1:I:208:ILE:HG22	2.40	0.52
2:L:73:LEU:HA	2:L:76:MET:HE3	1.92	0.52
1:E:238:GLU:N	1:E:238:GLU:OE1	2.44	0.51
1:E:181:TYR:HB2	1:E:201:ILE:HG23	1.92	0.51
1:G:186:LYS:NZ	1:G:190:GLU:O	2.44	0.51
1:E:163:ILE:CD1	1:G:206:TRP:CZ3	2.83	0.51
1:I:84:THR:OG1	1:I:119:THR:HG23	2.10	0.51
2:H:133:GLN:O	2:H:137:MET:HG3	2.10	0.51
1:M:208:ILE:HD12	1:O:161:HIS:CD2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:70:SER:OG	2:N:97:GLU:OE2	2.24	0.50
1:A:126:MET:SD	1:A:132:VAL:HG21	2.52	0.50
1:A:219:ILE:H	1:A:219:ILE:HD12	1.77	0.50
1:I:153:LEU:O	1:I:252:VAL:HG11	2.12	0.50
1:G:162:CYS:SG	1:G:209:LEU:HB2	2.52	0.49
1:A:190:GLU:HG3	1:A:191:ALA:N	2.28	0.49
1:C:62:LEU:HD11	2:D:87:LEU:HD21	1.95	0.49
1:O:187:LYS:CD	1:O:187:LYS:N	2.76	0.49
1:E:224:LEU:HD12	1:E:224:LEU:C	2.38	0.49
2:L:73:LEU:CD1	2:L:96:VAL:HG21	2.43	0.49
1:C:61:ILE:HD11	1:C:172:LEU:HD13	1.94	0.48
1:K:94:LYS:NZ	2:N:101:ASN:O	2.32	0.48
2:B:137:MET:O	2:B:138:ARG:C	2.56	0.48
1:M:61:ILE:HG13	1:M:62:LEU:H	1.78	0.48
2:N:29:ASP:OD2	2:N:91:ARG:HD2	2.13	0.48
1:M:53:THR:OG1	1:M:69:SER:O	2.32	0.48
2:P:99:LEU:HD13	2:P:107:PHE:CZ	2.48	0.48
2:H:106:TYR:OH	2:H:138:ARG:NH1	2.46	0.48
1:C:82:LEU:HD23	1:C:84:THR:HG23	1.94	0.48
1:E:171:ALA:O	2:F:91:ARG:NH2	2.46	0.48
2:H:48:SER:OG	3:H:201:SO4:O4	2.31	0.48
1:O:228:MET:CE	1:O:241:TYR:CD2	2.96	0.48
1:K:164:LEU:HD12	1:K:207:LEU:HD11	1.95	0.48
2:L:30:ILE:HG21	2:L:129:LEU:HB2	1.96	0.48
1:M:187:LYS:O	1:M:188:GLN:C	2.57	0.48
1:A:187:LYS:O	1:A:188:GLN:C	2.57	0.47
1:I:166:TRP:CZ3	1:I:207:LEU:HD12	2.49	0.47
1:O:82:LEU:HD12	1:O:93:HIS:O	2.15	0.47
1:G:187:LYS:H	1:G:187:LYS:HD2	1.79	0.47
2:H:98:VAL:O	2:H:102:ASN:ND2	2.47	0.47
1:G:134:LEU:N	1:G:134:LEU:HD22	2.28	0.47
1:K:214:LEU:HD22	1:K:256:ALA:HB2	1.97	0.47
1:O:182:GLU:O	1:O:224:LEU:HD12	2.14	0.47
1:A:161:HIS:NE2	3:A:301:SO4:O4	2.48	0.47
1:K:96:ILE:HD12	1:K:96:ILE:H	1.79	0.47
1:E:147:LEU:HD11	1:E:226:VAL:HG13	1.96	0.47
2:P:64:CYS:O	2:P:64:CYS:SG	2.73	0.46
1:I:181:TYR:HB2	1:I:201:ILE:HG23	1.98	0.46
1:I:113:VAL:HG22	1:I:114:PRO:HD2	1.96	0.46
1:O:80:TRP:HA	1:O:97:LEU:HD23	1.97	0.46
2:B:99:LEU:HD13	2:B:107:PHE:CZ	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:208:ILE:HD12	1:O:161:HIS:HD2	1.81	0.46
2:N:98:VAL:O	2:N:102:ASN:ND2	2.48	0.46
1:E:153:LEU:HD21	1:E:252:VAL:HG13	1.98	0.46
1:M:180:SER:CB	1:M:202:VAL:HG12	2.46	0.46
1:A:133:SER:C	1:A:134:LEU:HD22	2.41	0.45
1:C:73:LEU:HD12	1:C:122:PHE:HZ	1.80	0.45
1:G:157:ILE:HD12	1:G:256:ALA:HB2	1.97	0.45
1:K:153:LEU:HD21	1:K:250:GLN:O	2.16	0.45
1:O:182:GLU:C	1:O:224:LEU:HD12	2.41	0.45
1:A:168:ILE:C	1:A:168:ILE:HD12	2.41	0.45
2:P:65:THR:HG23	2:P:66:ARG:CG	2.45	0.45
1:C:54:PHE:HE1	1:C:97:LEU:HD21	1.82	0.45
1:C:210:GLU:O	1:C:211:ALA:CB	2.65	0.45
1:O:189:GLU:O	1:O:190:GLU:CB	2.65	0.45
1:G:129:ARG:O	1:G:129:ARG:HD3	2.17	0.45
1:G:255:GLN:HG2	1:G:256:ALA:H	1.81	0.45
2:B:136:LYS:C	2:B:138:ARG:H	2.25	0.45
2:H:55:LEU:CD2	2:H:79:THR:HG22	2.47	0.45
1:M:180:SER:HA	1:M:202:VAL:HG12	1.99	0.45
1:M:116:ASP:OD2	2:N:94:LYS:NZ	2.50	0.44
1:M:171:ALA:HA	2:N:88:ILE:HD11	1.99	0.44
1:A:171:ALA:HA	2:B:88:ILE:HD11	2.00	0.44
1:G:135:VAL:HG22	1:G:136:ASP:N	2.32	0.44
1:K:163:ILE:HD12	1:K:208:ILE:HG22	2.00	0.44
1:A:61:ILE:HD12	1:A:62:LEU:N	2.32	0.44
1:G:61:ILE:HD12	1:G:62:LEU:HB2	1.99	0.44
1:G:187:LYS:O	1:G:188:GLN:C	2.60	0.44
2:H:81:MET:HE2	2:H:81:MET:HB3	1.89	0.44
1:K:179:LEU:O	1:K:202:VAL:HG13	2.17	0.44
1:A:61:ILE:HD12	1:A:62:LEU:HB2	2.00	0.44
2:H:67:PRO:HA	2:H:113:CYS:SG	2.58	0.44
2:L:133:GLN:O	2:L:137:MET:HG3	2.18	0.44
1:M:214:LEU:HD13	1:M:256:ALA:HB1	2.00	0.43
1:I:82:LEU:HB3	1:I:121:THR:OG1	2.18	0.43
1:G:97:LEU:HD13	1:G:102:CYS:HB3	2.00	0.43
2:J:29:ASP:OD2	2:J:91:ARG:CD	2.66	0.43
1:O:255:GLN:O	1:O:256:ALA:C	2.60	0.43
1:A:113:VAL:HG13	1:A:114:PRO:HD2	1.98	0.43
1:A:130:GLU:O	1:A:132:VAL:HG23	2.18	0.43
2:D:29:ASP:OD2	2:D:91:ARG:HD2	2.18	0.43
1:G:153:LEU:O	1:G:252:VAL:HG11	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:61:ILE:HG22	2:L:87:LEU:HD21	1.99	0.43
1:O:189:GLU:O	1:O:190:GLU:HB2	2.19	0.43
1:E:53:THR:OG1	1:E:69:SER:O	2.30	0.43
1:M:117:ASN:OD1	1:M:117:ASN:O	2.37	0.43
2:B:61:SER:C	2:B:63:ASN:H	2.26	0.43
1:K:134:LEU:N	1:K:134:LEU:HD22	2.34	0.43
2:L:72:ARG:O	2:L:76:MET:HG3	2.19	0.43
1:G:111:VAL:HG22	2:H:87:LEU:CD1	2.49	0.42
2:N:99:LEU:HD13	2:N:107:PHE:CZ	2.54	0.42
1:A:50:ARG:O	1:A:53:THR:OG1	2.35	0.42
1:O:153:LEU:O	1:O:252:VAL:HG11	2.18	0.42
1:A:169:SER:HB3	2:D:39:GLU:OE2	2.19	0.42
2:B:57:LEU:HD13	2:B:76:MET:CE	2.49	0.42
1:E:80:TRP:HB3	1:E:96:ILE:HG22	2.01	0.42
1:G:111:VAL:HG22	2:H:87:LEU:HD12	2.01	0.42
1:K:187:LYS:C	1:K:189:GLU:N	2.78	0.42
1:K:216:PRO:HA	1:K:256:ALA:HB2	2.00	0.42
1:M:198:ARG:NH2	1:M:213:GLU:OE1	2.52	0.42
1:C:96:ILE:HD12	1:C:96:ILE:N	2.35	0.42
1:I:134:LEU:HD22	1:I:134:LEU:N	2.34	0.42
1:K:216:PRO:HA	1:K:256:ALA:CB	2.50	0.42
1:M:228:MET:HG2	1:M:241:TYR:CG	2.55	0.42
1:O:171:ALA:HA	2:P:88:ILE:HD11	2.01	0.42
1:A:169:SER:CB	2:D:39:GLU:OE2	2.67	0.42
1:C:191:ALA:HB3	1:C:194:GLN:OE1	2.19	0.42
1:C:214:LEU:HD23	1:C:256:ALA:HA	2.02	0.42
2:F:85:TYR:HB3	2:F:88:ILE:HD12	2.01	0.42
1:G:96:ILE:HD12	1:G:96:ILE:N	2.35	0.42
1:I:181:TYR:CD2	1:I:224:LEU:HD21	2.41	0.42
1:K:181:TYR:CD1	1:K:226:VAL:HG23	2.54	0.42
2:L:55:LEU:CD2	2:L:79:THR:HG22	2.50	0.42
1:O:96:ILE:HD12	1:O:96:ILE:N	2.35	0.42
1:A:98:ARG:HE	1:A:98:ARG:HA	1.84	0.42
1:A:236:VAL:HG12	1:A:237:GLU:N	2.34	0.42
1:G:187:LYS:O	1:G:187:LYS:HG2	2.19	0.42
2:H:41:PRO:HA	2:H:44:LYS:HG2	2.00	0.42
2:L:73:LEU:HD23	2:L:76:MET:HE3	2.01	0.42
1:K:87:GLN:O	1:M:92:THR:HG21	2.20	0.42
1:M:186:LYS:CD	1:M:190:GLU:HB2	2.50	0.42
1:O:207:LEU:C	1:O:207:LEU:HD12	2.45	0.42
2:P:81:MET:HE1	2:P:121:ALA:HB1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:153:LEU:O	1:C:252:VAL:HG11	2.19	0.41
2:D:32:PHE:CE1	2:D:36:LYS:HE3	2.55	0.41
1:A:233:ASP:O	1:A:235:VAL:N	2.46	0.41
2:F:55:LEU:HD23	2:F:79:THR:HG22	2.02	0.41
1:K:96:ILE:HD12	1:K:96:ILE:N	2.34	0.41
1:A:153:LEU:HD13	1:A:224:LEU:CD2	2.51	0.41
1:A:191:ALA:HB3	1:A:194:GLN:OE1	2.20	0.41
1:K:207:LEU:HD12	1:K:207:LEU:C	2.45	0.41
2:N:99:LEU:HD13	2:N:107:PHE:CE2	2.55	0.41
1:E:147:LEU:HD12	1:E:148:ASP:O	2.21	0.41
1:C:207:LEU:C	1:C:207:LEU:HD12	2.46	0.41
2:N:72:ARG:HH21	2:N:116:THR:HG21	1.85	0.41
1:O:187:LYS:N	1:O:187:LYS:HD2	2.35	0.41
2:P:63:ASN:O	2:P:63:ASN:ND2	2.53	0.41
1:A:255:GLN:O	1:A:256:ALA:C	2.63	0.41
2:J:81:MET:HE1	2:J:121:ALA:HB1	2.02	0.41
1:O:134:LEU:N	1:O:134:LEU:HD22	2.36	0.41
2:P:81:MET:HE2	2:P:81:MET:HB3	2.00	0.41
1:E:119:THR:HA	1:E:137:PRO:O	2.21	0.41
1:K:81:LEU:HG	1:K:120:ILE:CG2	2.51	0.41
1:O:140:LEU:HD22	1:O:142:ARG:NH1	2.36	0.41
1:C:82:LEU:HD21	1:C:92:THR:HG23	2.02	0.41
1:C:147:LEU:HD22	1:C:172:LEU:HD21	2.02	0.41
1:E:61:ILE:O	1:E:62:LEU:HG	2.20	0.41
1:I:163:ILE:HD12	1:I:208:ILE:HG22	2.03	0.41
1:I:181:TYR:CD2	1:I:226:VAL:HG22	2.55	0.41
1:K:83:PHE:O	1:K:92:THR:HA	2.21	0.41
1:O:96:ILE:HD12	1:O:96:ILE:H	1.85	0.41
1:O:113:VAL:HG13	1:O:114:PRO:HD2	2.02	0.41
1:A:233:ASP:N	1:A:233:ASP:OD1	2.54	0.41
2:D:128:LEU:O	2:D:131:ILE:HG22	2.21	0.41
1:E:142:ARG:HH21	1:E:240:ARG:N	2.19	0.41
1:M:61:ILE:HD12	1:M:62:LEU:HB2	2.03	0.41
1:A:153:LEU:HD21	1:A:250:GLN:O	2.21	0.40
2:B:59:ILE:CD1	2:B:119:GLY:HA3	2.51	0.40
1:E:105:VAL:O	1:E:105:VAL:HG23	2.21	0.40
1:E:53:THR:OG1	1:E:53:THR:O	2.37	0.40
1:K:119:THR:HA	1:K:137:PRO:O	2.21	0.40
2:N:57:LEU:HD12	2:N:121:ALA:HA	2.03	0.40
2:H:33:LEU:O	2:H:37:MET:HG2	2.21	0.40
1:M:174:PRO:HG2	2:N:88:ILE:HD12	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:113:VAL:HG13	1:G:114:PRO:HD2	2.03	0.40
1:I:224:LEU:C	1:I:224:LEU:HD23	2.46	0.40
2:B:59:ILE:N	2:B:59:ILE:HD12	2.36	0.40
1:C:113:VAL:HG13	1:C:114:PRO:HD2	2.03	0.40
1:C:135:VAL:HG22	1:C:136:ASP:N	2.36	0.40
1:I:96:ILE:N	1:I:96:ILE:HD12	2.36	0.40
1:M:92:THR:O	1:M:92:THR:HG23	2.22	0.40
2:N:55:LEU:HD23	2:N:79:THR:HG22	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:83:THR:O	2:L:84:ARG:HH21[2_644]	1.59	0.01

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	204/226 (90%)	189 (93%)	15 (7%)	0	100	100
1	C	204/226 (90%)	188 (92%)	14 (7%)	2 (1%)	12	41
1	E	164/226 (73%)	154 (94%)	8 (5%)	2 (1%)	10	37
1	G	192/226 (85%)	180 (94%)	10 (5%)	2 (1%)	12	41
1	I	170/226 (75%)	160 (94%)	9 (5%)	1 (1%)	21	52
1	K	180/226 (80%)	169 (94%)	9 (5%)	2 (1%)	11	39
1	M	193/226 (85%)	183 (95%)	9 (5%)	1 (0%)	24	57
1	O	178/226 (79%)	165 (93%)	13 (7%)	0	100	100
2	B	117/130 (90%)	111 (95%)	5 (4%)	1 (1%)	14	44
2	D	112/130 (86%)	107 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	117/130 (90%)	113 (97%)	4 (3%)	0	100	100
2	H	117/130 (90%)	110 (94%)	7 (6%)	0	100	100
2	J	117/130 (90%)	108 (92%)	9 (8%)	0	100	100
2	L	119/130 (92%)	116 (98%)	3 (2%)	0	100	100
2	N	117/130 (90%)	110 (94%)	6 (5%)	1 (1%)	14	44
2	P	113/130 (87%)	109 (96%)	4 (4%)	0	100	100
All	All	2414/2848 (85%)	2272 (94%)	130 (5%)	12 (0%)	24	57

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	188	GLN
1	I	188	GLN
1	K	188	GLN
1	M	188	GLN
2	B	137	MET
1	C	188	GLN
1	G	233	ASP
1	E	62	LEU
1	E	137	PRO
1	K	256	ALA
1	C	256	ALA
2	N	112	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	186/200 (93%)	186 (100%)	0	100	100
1	C	185/200 (92%)	185 (100%)	0	100	100
1	E	161/200 (80%)	160 (99%)	1 (1%)	78	83
1	G	180/200 (90%)	180 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	168/200 (84%)	168 (100%)	0	100	100
1	K	169/200 (84%)	168 (99%)	1 (1%)	78	83
1	M	181/200 (90%)	181 (100%)	0	100	100
1	O	170/200 (85%)	170 (100%)	0	100	100
2	B	110/118 (93%)	110 (100%)	0	100	100
2	D	106/118 (90%)	106 (100%)	0	100	100
2	F	110/118 (93%)	110 (100%)	0	100	100
2	H	110/118 (93%)	110 (100%)	0	100	100
2	J	110/118 (93%)	110 (100%)	0	100	100
2	L	111/118 (94%)	111 (100%)	0	100	100
2	N	110/118 (93%)	110 (100%)	0	100	100
2	P	108/118 (92%)	108 (100%)	0	100	100
All	All	2275/2544 (89%)	2273 (100%)	2 (0%)	88	90

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	102	CYS
1	K	102	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	GLN
1	A	124	HIS
1	C	60	ASN
1	C	197	HIS
1	C	244	GLN
2	D	38	GLN
2	F	35	ASN
2	F	111	GLN
1	G	60	ASN
1	G	87	GLN
2	H	46	HIS
1	I	144	HIS
1	I	197	HIS
1	I	244	GLN

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Mol	Chain	Res	Type
2	J	35	ASN
1	K	60	ASN
1	K	87	GLN
1	K	188	GLN
2	L	102	ASN
2	L	111	GLN
2	L	115	GLN
1	M	197	HIS
2	N	46	HIS
1	O	60	ASN
1	O	144	HIS
2	P	63	ASN

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](#)

10 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	$\# Z > 2$
3	SO4	J	201	-	4,4,4	0.23	0	6,6,6	0.07	0
3	SO4	F	201	-	4,4,4	0.24	0	6,6,6	0.06	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	G	301	-	4,4,4	0.23	0	6,6,6	0.07	0
3	SO4	B	201	-	4,4,4	0.24	0	6,6,6	0.08	0
3	SO4	A	301	-	4,4,4	0.22	0	6,6,6	0.18	0
3	SO4	N	201	-	4,4,4	0.23	0	6,6,6	0.07	0
3	SO4	O	301	-	4,4,4	0.22	0	6,6,6	0.12	0
3	SO4	I	301	-	4,4,4	0.23	0	6,6,6	0.08	0
3	SO4	H	201	-	4,4,4	0.24	0	6,6,6	0.10	0
3	SO4	D	201	-	4,4,4	0.24	0	6,6,6	0.07	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.

7 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	J	201	SO4	2	0
3	G	301	SO4	4	0
3	B	201	SO4	2	0
3	A	301	SO4	2	0
3	O	301	SO4	5	0
3	H	201	SO4	1	0
3	D	201	SO4	2	0

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	208/226 (92%)	-0.51	0 100 100	68, 111, 176, 211	0
1	C	206/226 (91%)	-0.55	0 100 100	66, 108, 181, 263	0
1	E	176/226 (77%)	-0.46	0 100 100	105, 158, 210, 236	0
1	G	198/226 (87%)	-0.61	0 100 100	85, 123, 189, 256	0
1	I	182/226 (80%)	-0.40	0 100 100	109, 156, 211, 261	0
1	K	188/226 (83%)	-0.49	0 100 100	105, 142, 211, 259	0
1	M	199/226 (88%)	-0.45	0 100 100	91, 134, 204, 256	0
1	O	188/226 (83%)	-0.52	0 100 100	84, 133, 182, 225	0
2	B	119/130 (91%)	-0.49	0 100 100	77, 112, 174, 210	0
2	D	116/130 (89%)	-0.58	0 100 100	77, 112, 175, 218	0
2	F	119/130 (91%)	-0.56	0 100 100	97, 131, 183, 234	0
2	H	119/130 (91%)	-0.54	0 100 100	76, 103, 149, 174	0
2	J	119/130 (91%)	-0.48	0 100 100	106, 140, 204, 236	0
2	L	121/130 (93%)	-0.47	0 100 100	110, 144, 198, 236	0
2	N	119/130 (91%)	-0.52	0 100 100	85, 120, 178, 208	0
2	P	117/130 (90%)	-0.46	0 100 100	100, 148, 201, 238	0
All	All	2494/2848 (87%)	-0.50	0 100 100	66, 132, 198, 263	0

There are no RSRZ outliers to report.

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

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	G	301	5/5	0.77	0.08	141,154,164,171	0
3	SO4	F	201	5/5	0.80	0.08	130,130,148,152	0
3	SO4	D	201	5/5	0.82	0.09	134,134,141,147	0
3	SO4	H	201	5/5	0.84	0.09	108,129,147,156	0
3	SO4	B	201	5/5	0.85	0.07	110,110,134,140	0
3	SO4	J	201	5/5	0.86	0.07	118,128,132,139	0
3	SO4	N	201	5/5	0.89	0.06	124,138,140,141	0
3	SO4	A	301	5/5	0.90	0.08	132,137,143,156	0
3	SO4	I	301	5/5	0.90	0.07	145,159,168,169	0
3	SO4	O	301	5/5	0.91	0.08	139,142,149,155	0

6.5 Other polymers [i](#)

There are no such residues in this entry.