



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 05:56 AM GMT

PDB ID : 3MKP
Title : Crystal structure of 1K1 mutant of Hepatocyte Growth Factor/Scatter Factor fragment NK1 in complex with heparin
Authors : Gherardi, E.; Chirgadze, D.Y.; Blundell, T.L.
Deposited on : 2010-04-15
Resolution : 2.81 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

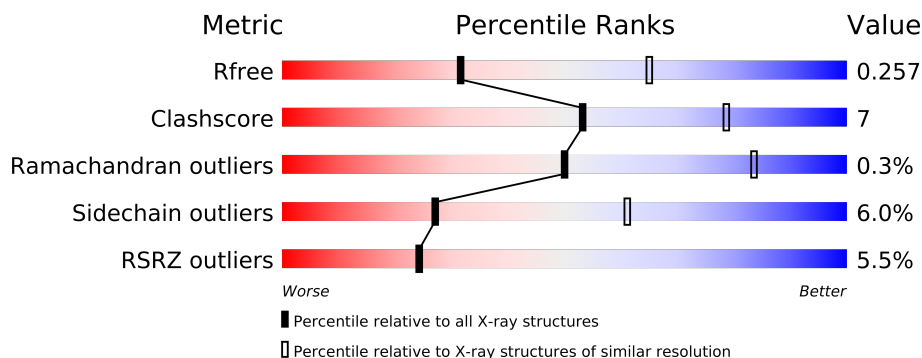
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.81 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}	66092	1963 (2.84-2.80)
Clashscore	79885	2478 (2.84-2.80)
Ramachandran outliers	78287	2429 (2.84-2.80)
Sidechain outliers	78261	2431 (2.84-2.80)
RSRZ outliers	66119	1966 (2.84-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	183	
1	B	183	
1	C	183	
1	D	183	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	SGN	A	3	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5766 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Hepatocyte growth factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	173	Total	C	N	O	S	0	0	0
			1380	868	242	258	12			
1	B	173	Total	C	N	O	S	0	0	0
			1378	869	241	256	12			
1	C	173	Total	C	N	O	S	0	0	0
			1376	867	243	254	12			
1	D	169	Total	C	N	O	S	0	0	0
			1327	834	233	248	12			

There are 8 discrepancies between the modelled and reference sequences:

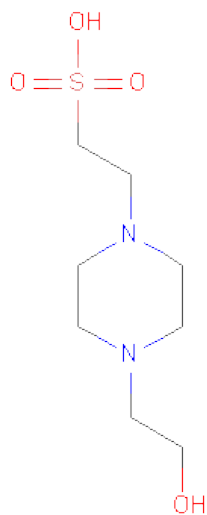
Chain	Residue	Modelled	Actual	Comment	Reference
A	132	GLU	LYS	ENGINEERED MUTATION	UNP P14210
A	134	GLU	ARG	ENGINEERED MUTATION	UNP P14210
B	132	GLU	LYS	ENGINEERED MUTATION	UNP P14210
B	134	GLU	ARG	ENGINEERED MUTATION	UNP P14210
C	132	GLU	LYS	ENGINEERED MUTATION	UNP P14210
C	134	GLU	ARG	ENGINEERED MUTATION	UNP P14210
D	132	GLU	LYS	ENGINEERED MUTATION	UNP P14210
D	134	GLU	ARG	ENGINEERED MUTATION	UNP P14210

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



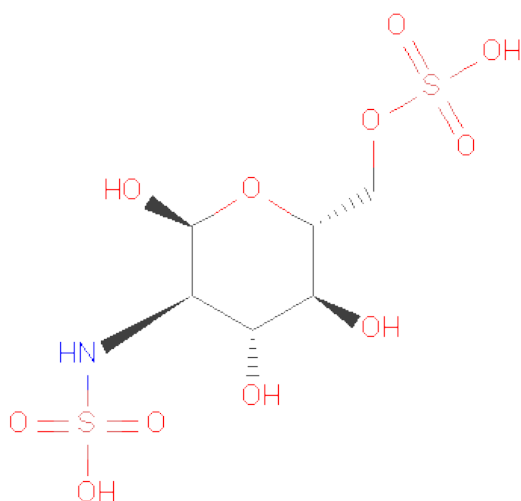
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is 4-(2-HYDROXYETHYL)-1-PIPERAZINEETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 4 is SUGAR (N,O6-DISULFO-GLUCOSAMINE) (three-letter code: SGN) (formula: C₆H₁₃NO₁₁S₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			19	6	1	10	2		

- Molecule 5 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	6	Total	C	N	O	S	0	0
			105	36	3	57	9		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	132	GLU	LYS	ENGINEERED MUTATION	UNP P14210
C	134	GLU	ARG	ENGINEERED MUTATION	UNP P14210

- Molecule 6 is water.

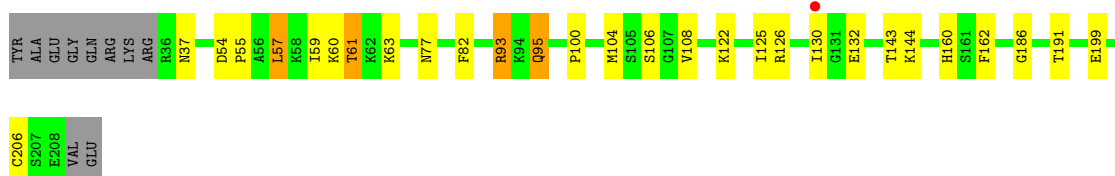
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	31	Total 31	O 31	0	0
6	B	25	Total 25	O 25	0	0
6	C	15	Total 15	O 15	0	0
6	D	30	Total 30	O 30	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

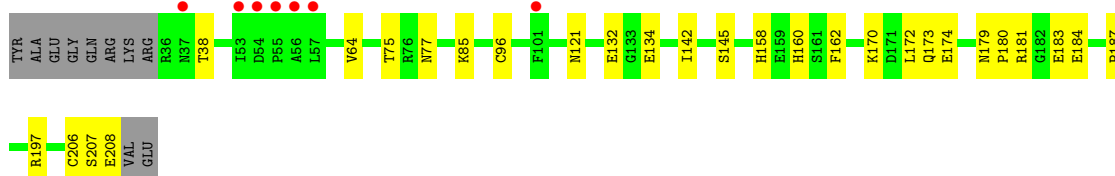
- Molecule 1: Hepatocyte growth factor

Chain A: 



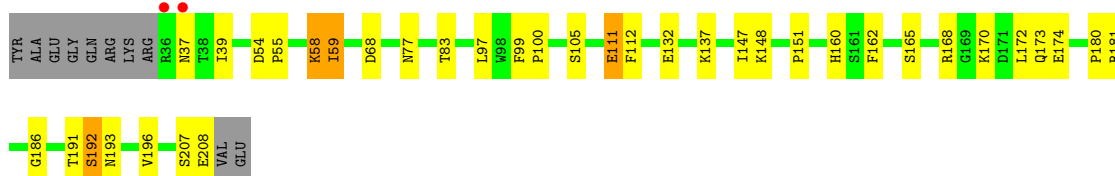
- Molecule 1: Hepatocyte growth factor

Chain B: 



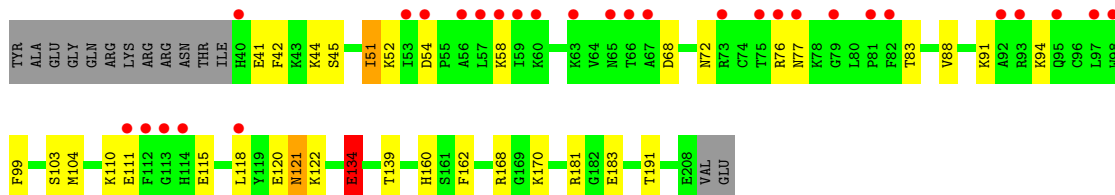
- Molecule 1: Hepatocyte growth factor

Chain C: 



- Molecule 1: Hepatocyte growth factor

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	129.73Å 129.73Å 118.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.69 – 2.81 49.68 – 2.81	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.69-2.81) 99.8 (49.68-2.81)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.26 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.199 , 0.261 0.198 , 0.257	Depositor DCC
R_{free} test set	1287 reflections (5.38%)	DCC
Wilson B-factor (Å ²)	43.1	Xtriage
Anisotropy	0.135	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 1.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 25194 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	5766	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.84% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, EPE, IDS, SGN

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	0.53	0/1415	0.64	0/1907
1	B	0.54	0/1413	0.62	0/1903
1	C	0.53	0/1411	0.58	0/1901
1	D	0.57	0/1360	0.61	0/1827
All	All	0.54	0/5599	0.61	0/7538

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1380	0	1321	16	0
1	B	1378	0	1328	17	0
1	C	1376	0	1324	24	0
1	D	1327	0	1256	20	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	15	0	17	0	0
3	B	15	0	17	0	0
3	C	15	0	17	0	0
3	D	15	0	17	0	0
4	A	19	0	10	3	0
5	C	105	0	45	1	77
6	A	31	0	0	1	0
6	B	25	0	0	0	0
6	C	15	0	0	1	0
6	D	30	0	0	0	0
All	All	5766	0	5352	77	77

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

All (77) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:172:LEU:HD21	1:B:180:PRO:HG3	1.47	0.96
1:C:147:ILE:HG21	1:C:191:THR:HG23	1.45	0.96
1:A:160:HIS:HD2	1:A:162:PHE:H	1.23	0.83
1:D:51:ILE:HD11	1:D:111:GLU:HB2	1.65	0.76
1:D:160:HIS:HD2	1:D:162:PHE:H	1.31	0.75
1:B:160:HIS:HD2	1:B:162:PHE:H	1.31	0.75
1:A:61:THR:N	4:A:3:SGN:O1S	2.23	0.72
1:C:162:PHE:HE1	1:C:181:ARG:HD2	1.54	0.71
1:A:54:ASP:HB3	1:A:57:LEU:HD22	1.71	0.70
1:C:148:LYS:O	1:C:192:SER:HB2	1.92	0.70
1:C:172:LEU:HD21	1:C:180:PRO:HG3	1.75	0.69
1:A:93:ARG:NH1	1:A:95:GLN:OE1	2.27	0.68
1:D:88:VAL:HG23	1:D:99:PHE:HE2	1.59	0.66
1:A:144:LYS:HE3	6:A:17:HOH:O	1.97	0.64
1:C:147:ILE:CG2	1:C:191:THR:HG23	2.23	0.64
1:A:160:HIS:HD2	1:A:162:PHE:N	1.95	0.63
1:B:132:GLU:OE2	1:B:132:GLU:HA	1.98	0.62
1:C:151:PRO:HD3	6:C:218:HOH:O	2.01	0.61
1:B:160:HIS:CD2	1:B:162:PHE:H	2.16	0.61
1:C:58:LYS:HE3	1:C:58:LYS:HA	1.84	0.59
1:C:191:THR:HG22	1:C:193:ASN:H	1.68	0.59
1:D:88:VAL:HG23	1:D:99:PHE:CE2	2.37	0.57
1:C:132:GLU:O	1:C:186:GLY:HA2	2.03	0.57
1:D:160:HIS:CD2	1:D:162:PHE:H	2.19	0.57
1:A:130:ILE:HD11	1:B:206:CYS:O	2.05	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:160:HIS:CD2	1:A:162:PHE:H	2.13	0.56
1:D:121:ASN:C	1:D:121:ASN:OD1	2.44	0.56
1:B:134:GLU:OE2	1:B:170:LYS:HE3	2.05	0.56
1:D:122:LYS:HE2	1:D:139:THR:HG21	1.88	0.56
1:C:147:ILE:HG21	1:C:191:THR:CG2	2.28	0.56
1:B:160:HIS:HD2	1:B:162:PHE:N	2.01	0.55
1:D:103:SER:HB3	1:D:110:LYS:HE2	1.88	0.55
1:C:162:PHE:CE1	1:C:181:ARG:HD2	2.41	0.54
1:D:134:GLU:OE1	1:D:170:LYS:HE3	2.08	0.53
1:D:72:ASN:O	1:D:76:ARG:HG3	2.07	0.53
1:C:191:THR:HG22	1:C:193:ASN:N	2.23	0.53
1:A:122:LYS:HA	1:A:125:ILE:HD12	1.91	0.52
1:D:44:LYS:HG2	1:D:45:SER:N	2.24	0.52
1:B:132:GLU:OE1	1:B:184:GLU:HA	2.10	0.52
1:B:158:HIS:CD2	1:B:197:ARG:HA	2.45	0.52
1:A:63:LYS:HG2	4:A:3:SGN:O4S	2.11	0.51
1:C:207:SER:O	1:C:208:GLU:CB	2.60	0.50
5:C:4:SGN:H61	5:C:5:IDS:C1	2.41	0.50
1:A:60:LYS:HA	4:A:3:SGN:O1S	2.12	0.50
1:D:42:PHE:HA	1:D:120:GLU:O	2.13	0.48
1:B:38:THR:HG21	1:B:75:THR:HG21	1.96	0.48
1:A:143:THR:HB	1:A:199:GLU:HB3	1.97	0.47
1:A:132:GLU:O	1:A:186:GLY:HA2	2.14	0.47
1:D:68:ASP:O	1:D:72:ASN:ND2	2.47	0.47
1:B:158:HIS:NE2	1:B:197:ARG:HA	2.30	0.47
1:C:59:ILE:HD11	1:C:99:PHE:HE1	1.80	0.47
1:D:91:LYS:HG2	1:D:115:GLU:O	2.16	0.46
1:B:181:ARG:HB2	1:B:183:GLU:HG3	1.98	0.46
1:D:45:SER:HB2	1:D:118:LEU:HB3	1.97	0.45
1:B:207:SER:O	1:B:208:GLU:CB	2.64	0.45
1:C:191:THR:CG2	1:C:193:ASN:H	2.30	0.45
1:C:83:THR:O	1:C:100:PRO:HA	2.17	0.45
1:C:111:GLU:HG3	1:C:112:PHE:N	2.31	0.45
1:C:191:THR:HB	1:C:196:VAL:O	2.16	0.44
1:C:207:SER:O	1:C:208:GLU:HB2	2.17	0.44
1:D:41:GLU:HA	1:D:122:LYS:HE3	1.99	0.44
1:B:64:VAL:HG21	1:B:96:CYS:SG	2.58	0.44
1:C:54:ASP:HA	1:C:55:PRO:HD3	1.88	0.44
1:C:170:LYS:HE2	1:C:180:PRO:O	2.18	0.43
1:A:54:ASP:HA	1:A:55:PRO:HD3	1.89	0.43
1:A:82:PHE:HB2	1:A:100:PRO:HB3	2.00	0.43
1:B:85:LYS:O	1:B:121:ASN:HB3	2.19	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:103:SER:CB	1:D:110:LYS:HE2	2.47	0.42
1:C:160:HIS:HD2	1:C:162:PHE:N	2.17	0.42
1:B:173:GLN:O	1:B:174:GLU:C	2.58	0.42
1:B:179:ASN:HB2	1:B:187:PRO:HA	2.01	0.42
1:C:37:ASN:HD22	1:C:39:ILE:HG22	1.84	0.41
1:D:41:GLU:OE2	1:D:41:GLU:CA	2.68	0.41
1:C:173:GLN:O	1:C:174:GLU:C	2.57	0.41
1:D:181:ARG:HB2	1:D:183:GLU:HG3	2.02	0.41
1:D:121:ASN:OD1	1:D:122:LYS:N	2.54	0.40
1:A:126:ARG:HD3	1:A:206:CYS:SG	2.62	0.40

All (77) 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	Distance(Å)	Clash(Å)
5:C:4:SGN:O5S	5:C:5:IDS:O2S[8_554]	0.32	1.88
5:C:212:IDS:C5	5:C:6:SGN:O5[8_554]	0.62	1.58
5:C:4:SGN:S2	5:C:5:IDS:O3S[8_554]	0.75	1.45
5:C:212:IDS:C4	5:C:6:SGN:C1[8_554]	0.79	1.41
5:C:212:IDS:C5	5:C:6:SGN:C5[8_554]	0.80	1.40
5:C:4:SGN:S2	5:C:5:IDS:S[8_554]	0.83	1.37
5:C:4:SGN:C6	5:C:5:IDS:O2[8_554]	0.86	1.34
5:C:4:SGN:O5	5:C:5:IDS:C3[8_554]	0.98	1.22
5:C:4:SGN:O6	5:C:5:IDS:O2[8_554]	0.98	1.22
5:C:212:IDS:C4	5:C:6:SGN:O5[8_554]	0.99	1.21
5:C:4:SGN:C1	5:C:5:IDS:C4[8_554]	1.06	1.14
5:C:4:SGN:C5	5:C:5:IDS:C2[8_554]	1.16	1.04
5:C:212:IDS:C6	5:C:6:SGN:C5[8_554]	1.20	1.00
5:C:4:SGN:O6	5:C:5:IDS:S[8_554]	1.23	0.97
5:C:4:SGN:O4S	5:C:5:IDS:O3S[8_554]	1.24	0.96
5:C:4:SGN:O5S	5:C:5:IDS:S[8_554]	1.25	0.95
5:C:212:IDS:O5	5:C:6:SGN:C6[8_554]	1.26	0.94
5:C:4:SGN:C4	5:C:5:IDS:C1[8_554]	1.26	0.94
5:C:4:SGN:O6S	5:C:5:IDS:O3S[8_554]	1.26	0.94
5:C:4:SGN:C2	5:C:5:IDS:O3[8_554]	1.27	0.93
5:C:4:SGN:C6	5:C:5:IDS:C2[8_554]	1.34	0.86
5:C:4:SGN:O5	5:C:5:IDS:C4[8_554]	1.37	0.83
5:C:4:SGN:C5	5:C:5:IDS:C1[8_554]	1.48	0.72
5:C:4:SGN:C5	5:C:5:IDS:C3[8_554]	1.50	0.70
5:C:4:SGN:O6	5:C:5:IDS:C2[8_554]	1.52	0.68
5:C:4:SGN:C1	5:C:5:IDS:C3[8_554]	1.53	0.67
5:C:4:SGN:C4	5:C:5:IDS:C2[8_554]	1.56	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:C:212:IDS:O4	5:C:6:SGN:C1[8_554]	1.57	0.63
5:C:212:IDS:O5	5:C:6:SGN:O5[8_554]	1.57	0.63
5:C:212:IDS:O5	5:C:6:SGN:C5[8_554]	1.58	0.62
5:C:4:SGN:C5	5:C:5:IDS:O5[8_554]	1.58	0.62
5:C:4:SGN:O5	5:C:5:IDS:O4[8_554]	1.63	0.57
5:C:4:SGN:C3	5:C:5:IDS:O3[8_554]	1.68	0.52
5:C:4:SGN:S2	5:C:5:IDS:O2S[8_554]	1.68	0.52
5:C:212:IDS:O62	5:C:6:SGN:C3[8_554]	1.70	0.50
5:C:4:SGN:C5	5:C:5:IDS:C4[8_554]	1.70	0.50
5:C:212:IDS:C5	5:C:6:SGN:C1[8_554]	1.72	0.48
5:C:4:SGN:C6	5:C:5:IDS:C1[8_554]	1.74	0.46
5:C:4:SGN:O4	5:C:5:IDS:O5[8_554]	1.78	0.42
5:C:4:SGN:C2	5:C:5:IDS:C3[8_554]	1.79	0.41
5:C:4:SGN:C5	5:C:5:IDS:O2[8_554]	1.79	0.41
5:C:4:SGN:O6	5:C:5:IDS:O3S[8_554]	1.79	0.41
5:C:4:SGN:C4	5:C:5:IDS:C3[8_554]	1.81	0.39
5:C:4:SGN:C3	5:C:5:IDS:C5[8_554]	1.82	0.38
5:C:4:SGN:O5	5:C:5:IDS:C2[8_554]	1.82	0.38
5:C:4:SGN:C1	5:C:5:IDS:O4[8_554]	1.83	0.37
5:C:4:SGN:O4S	5:C:5:IDS:S[8_554]	1.83	0.37
5:C:4:SGN:C2	5:C:5:IDS:C4[8_554]	1.84	0.36
5:C:4:SGN:C4	5:C:5:IDS:O5[8_554]	1.90	0.30
5:C:4:SGN:C5	5:C:5:IDS:C5[8_554]	1.92	0.28
5:C:212:IDS:C3	5:C:6:SGN:O5[8_554]	1.93	0.27
5:C:4:SGN:O4S	5:C:5:IDS:O1S[8_554]	1.94	0.26
5:C:212:IDS:C5	5:C:6:SGN:C4[8_554]	1.95	0.25
5:C:212:IDS:C5	5:C:6:SGN:C6[8_554]	1.95	0.25
5:C:212:IDS:C6	5:C:6:SGN:O5[8_554]	1.95	0.25
5:C:212:IDS:O61	5:C:6:SGN:C5[8_554]	1.96	0.24
5:C:4:SGN:C4	5:C:5:IDS:O3[8_554]	1.97	0.23
5:C:212:IDS:C1	5:C:6:SGN:O5S[8_554]	1.98	0.22
5:C:4:SGN:C4	5:C:5:IDS:C5[8_554]	2.00	0.20
5:C:212:IDS:O4	5:C:6:SGN:O5[8_554]	2.02	0.18
5:C:212:IDS:O5	5:C:6:SGN:O6[8_554]	2.02	0.18
5:C:212:IDS:C1	5:C:6:SGN:O6[8_554]	2.04	0.16
5:C:4:SGN:S2	5:C:5:IDS:O1S[8_554]	2.04	0.16
5:C:4:SGN:O6	5:C:5:IDS:O1S[8_554]	2.05	0.15
5:C:212:IDS:C6	5:C:6:SGN:C4[8_554]	2.06	0.14
5:C:212:IDS:C4	5:C:6:SGN:C2[8_554]	2.07	0.13
5:C:4:SGN:O5	5:C:5:IDS:O2[8_554]	2.09	0.11
5:C:4:SGN:C3	5:C:5:IDS:C4[8_554]	2.13	0.07
5:C:4:SGN:S2	5:C:5:IDS:O2[8_554]	2.13	0.07

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:C:212:IDS:O62	5:C:6:SGN:C4[8_554]	2.14	0.06
5:C:4:SGN:O5S	5:C:5:IDS:O1S[8_554]	2.14	0.06
5:C:212:IDS:O62	5:C:6:SGN:C5[8_554]	2.15	0.05
5:C:4:SGN:C3	5:C:5:IDS:C3[8_554]	2.16	0.04
5:C:4:SGN:O5S	5:C:5:IDS:O3S[8_554]	2.16	0.04
5:C:212:IDS:C6	5:C:6:SGN:C1[8_554]	2.19	0.01
5:C:4:SGN:C5	5:C:5:IDS:O4[8_554]	2.19	0.01
5:C:4:SGN:O6S	5:C:5:IDS:S[8_554]	2.19	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	171/183 (93%)	165 (96%)	6 (4%)	0	100	100
1	B	171/183 (93%)	162 (95%)	9 (5%)	0	100	100
1	C	171/183 (93%)	157 (92%)	14 (8%)	0	100	100
1	D	167/183 (91%)	149 (89%)	16 (10%)	2 (1%)	19	53
All	All	680/732 (93%)	633 (93%)	45 (7%)	2 (0%)	50	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	134	GLU
1	D	54	ASP

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	153/164 (93%)	142 (93%)	11 (7%)	21	49
1	B	153/164 (93%)	150 (98%)	3 (2%)	68	93
1	C	152/164 (93%)	141 (93%)	11 (7%)	21	49
1	D	144/164 (88%)	133 (92%)	11 (8%)	19	46
All	All	602/656 (92%)	566 (94%)	36 (6%)	27	61

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

Mol	Chain	Res	Type
1	A	37	ASN
1	A	57	LEU
1	A	59	ILE
1	A	61	THR
1	A	77	ASN
1	A	93	ARG
1	A	95	GLN
1	A	104	MET
1	A	106	SER
1	A	108	VAL
1	A	191	THR
1	B	77	ASN
1	B	142	ILE
1	B	145	SER
1	C	58	LYS
1	C	59	ILE
1	C	68	ASP
1	C	77	ASN
1	C	97	LEU
1	C	105	SER
1	C	111	GLU
1	C	137	LYS
1	C	165	SER
1	C	168	ARG
1	C	192	SER
1	D	51	ILE
1	D	52	LYS
1	D	58	LYS
1	D	77	ASN
1	D	83	THR
1	D	94	LYS
1	D	104	MET
1	D	121	ASN

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Mol	Chain	Res	Type
1	D	134	GLU
1	D	168	ARG
1	D	191	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	72	ASN
1	A	160	HIS
1	B	72	ASN
1	B	160	HIS
1	C	37	ASN
1	C	72	ASN
1	C	160	HIS
1	C	205	GLN
1	D	158	HIS
1	D	160	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

6 carbohydrates 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
5	SGN	C	2	5	17,19,20	2.22	2 (11%)	24,29,31	1.43	4 (16%)
5	IDS	C	212	5	15,16,17	1.04	1 (6%)	20,24,26	0.87	1 (5%)
5	SGN	C	4	5	17,19,20	1.43	3 (17%)	24,29,31	1.40	4 (16%)
5	IDS	C	5	5	15,16,17	1.01	1 (6%)	20,24,26	0.93	1 (5%)
5	SGN	C	6	5	17,19,20	1.62	2 (11%)	24,29,31	1.27	4 (16%)
5	IDS	C	7	5	15,16,17	1.10	1 (6%)	20,24,26	0.98	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SGN	C	2	5	-	0/11/28/31	0/1/1/1
5	IDS	C	212	5	-	0/9/26/29	0/1/1/1
5	SGN	C	4	5	-	0/11/28/31	0/1/1/1
5	IDS	C	5	5	-	0/9/26/29	0/1/1/1
5	SGN	C	6	5	-	0/11/28/31	0/1/1/1
5	IDS	C	7	5	-	0/9/26/29	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	2	SGN	O1S-S1	6.47	1.48	1.42
5	C	2	SGN	O2S-S1	5.59	1.48	1.42
5	C	6	SGN	O1S-S1	4.37	1.46	1.42
5	C	6	SGN	O2S-S1	3.85	1.46	1.42
5	C	4	SGN	O2S-S1	3.70	1.46	1.42
5	C	4	SGN	O1S-S1	3.29	1.45	1.42
5	C	7	IDS	O2-S	2.67	1.64	1.60
5	C	212	IDS	O2-S	2.58	1.63	1.60
5	C	5	IDS	O2-S	2.44	1.63	1.60
5	C	4	SGN	C2-N	-2.19	1.45	1.48

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	2	SGN	C6-O6-S2	4.27	122.25	116.76
5	C	4	SGN	C6-O6-S2	3.87	121.73	116.76
5	C	4	SGN	O2S-S1-O1S	-2.99	110.52	119.84
5	C	5	IDS	C4-C3-C2	2.86	113.20	109.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	2	SGN	O2S-S1-O1S	-2.69	111.45	119.84
5	C	6	SGN	O2S-S1-N	-2.59	104.91	108.32
5	C	7	IDS	C4-C3-C2	2.54	112.76	109.29
5	C	212	IDS	C4-C3-C2	2.54	112.76	109.29
5	C	6	SGN	O3S-S1-O2S	-2.23	111.25	115.28
5	C	4	SGN	O2S-S1-N	-2.16	105.47	108.32
5	C	6	SGN	O3S-S1-O1S	-2.13	111.43	115.28
5	C	2	SGN	O3S-S1-O2S	-2.11	111.46	115.28
5	C	2	SGN	O3S-S1-O1S	-2.11	111.47	115.28
5	C	6	SGN	O2S-S1-O1S	-2.08	113.36	119.84
5	C	4	SGN	C2-N-S1	-2.02	118.67	122.34

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry ⓘ

9 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
2	SO4	A	1	-	4,4,4	0.21	0	6,6,6	0.43	0
3	EPE	A	211	-	15,15,15	0.77	1 (6%)	20,20,20	1.94	4 (20%)
4	SGN	A	3	-	17,19,20	1.72	2 (11%)	24,29,31	1.44	3 (12%)
2	SO4	B	2	-	4,4,4	0.30	0	6,6,6	0.09	0
3	EPE	B	211	-	15,15,15	0.80	1 (6%)	20,20,20	2.02	6 (30%)
3	EPE	C	211	-	15,15,15	0.77	1 (6%)	20,20,20	2.07	5 (25%)
2	SO4	C	3	-	4,4,4	0.12	0	6,6,6	0.33	0
3	EPE	D	211	-	15,15,15	0.80	1 (6%)	20,20,20	2.62	10 (50%)
2	SO4	D	4	-	4,4,4	0.15	0	6,6,6	0.26	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	1	-	-	0/0/0/0	0/0/0/0
3	EPE	A	211	-	-	0/9/19/19	0/1/1/1
4	SGN	A	3	-	-	0/11/28/31	0/1/1/1
2	SO4	B	2	-	-	0/0/0/0	0/0/0/0
3	EPE	B	211	-	-	0/9/19/19	0/1/1/1
3	EPE	C	211	-	-	0/9/19/19	0/1/1/1
2	SO4	C	3	-	-	0/0/0/0	0/0/0/0
3	EPE	D	211	-	-	0/9/19/19	0/1/1/1
2	SO4	D	4	-	-	0/0/0/0	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	3	SGN	O2S-S1	4.92	1.47	1.42
4	A	3	SGN	O1S-S1	4.00	1.46	1.42
3	B	211	EPE	C10-S	2.70	1.81	1.77
3	D	211	EPE	C10-S	2.54	1.81	1.77
3	C	211	EPE	C10-S	2.53	1.81	1.77
3	A	211	EPE	C10-S	2.42	1.81	1.77

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	211	EPE	O2S-S-C10	5.91	111.87	106.81
3	A	211	EPE	O3S-S-C10	5.74	113.19	105.93
3	D	211	EPE	O1S-S-C10	5.63	111.63	106.81
3	D	211	EPE	O2S-S-C10	5.07	111.15	106.81
3	C	211	EPE	C5-N4-C3	4.58	120.23	108.86
3	D	211	EPE	C5-N4-C3	4.18	119.23	108.86
3	C	211	EPE	O3S-S-C10	4.08	111.09	105.93
4	A	3	SGN	C6-O6-S2	3.92	121.81	116.76
3	C	211	EPE	O2S-S-C10	3.49	109.80	106.81
4	A	3	SGN	O1S-S1-N	-3.48	103.74	108.32
3	A	211	EPE	C5-N4-C3	3.45	117.44	108.86
3	B	211	EPE	C7-N4-C3	3.45	120.22	111.32
3	D	211	EPE	O3S-S-C10	3.41	110.25	105.93
3	C	211	EPE	C7-N4-C3	3.40	120.09	111.32
3	B	211	EPE	C5-N4-C3	3.26	116.97	108.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	211	EPE	C7-N4-C5	3.24	119.68	111.32
3	D	211	EPE	C7-N4-C3	3.19	119.57	111.32
3	D	211	EPE	C7-N4-C5	2.84	118.64	111.32
3	D	211	EPE	C9-N1-C6	-2.81	104.06	111.32
3	D	211	EPE	C2-C3-N4	2.73	115.98	110.61
3	B	211	EPE	C7-N4-C5	2.66	118.19	111.32
4	A	3	SGN	O2S-S1-O1S	-2.65	111.59	119.84
3	B	211	EPE	O3S-S-O2S	-2.49	106.39	111.78
3	A	211	EPE	C7-N4-C3	2.31	117.27	111.32
3	D	211	EPE	C3-C2-N1	2.27	115.08	110.61
3	D	211	EPE	O2S-S-O1S	-2.25	105.22	113.26
3	B	211	EPE	O3S-S-C10	2.20	108.71	105.93
3	A	211	EPE	O3S-S-O2S	-2.00	107.46	111.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 ⓘ

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	173/183 (94%)	-0.00	1 (0%) 86 88	5, 18, 40, 45	0
1	B	173/183 (94%)	0.07	7 (4%) 36 37	3, 22, 43, 62	0
1	C	173/183 (94%)	0.11	2 (1%) 75 76	7, 27, 48, 62	0
1	D	169/183 (92%)	0.67	29 (17%) 2 2	2, 30, 63, 69	0
All	All	688/732 (93%)	0.21	39 (5%) 24 22	2, 23, 59, 69	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	66	THR	6.4
1	B	57	LEU	6.3
1	D	58	LYS	5.0
1	B	56	ALA	4.0
1	D	95	GLN	4.0
1	D	97	LEU	3.9
1	B	54	ASP	3.9
1	D	76	ARG	3.8
1	D	57	LEU	3.8
1	D	112	PHE	3.5
1	D	82	PHE	3.4
1	C	36	ARG	3.4
1	B	53	ILE	3.3
1	D	79	GLY	3.2
1	D	113	GLY	3.1
1	D	59	ILE	3.0
1	D	81	PRO	2.9
1	D	92	ALA	2.9
1	D	40	HIS	2.9
1	D	65	ASN	2.9
1	D	77	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	63	LYS	2.8
1	D	98	TRP	2.7
1	D	73	ARG	2.6
1	C	37	ASN	2.6
1	D	75	THR	2.6
1	B	101	PHE	2.5
1	D	67	ALA	2.5
1	D	111	GLU	2.4
1	D	53	ILE	2.4
1	B	55	PRO	2.4
1	D	60	LYS	2.3
1	D	114	HIS	2.3
1	D	54	ASP	2.2
1	A	130	ILE	2.2
1	D	56	ALA	2.2
1	D	93	ARG	2.1
1	B	37	ASN	2.1
1	D	118	LEU	2.0

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 ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	SGN	C	2	19/20	0.33	3.45	63,68,73,73	19
5	IDS	C	212	16/17	0.26	2.91	46,56,64,65	16
5	IDS	C	7	16/17	0.21	0.16	46,52,56,58	16
5	IDS	C	5	16/17	0.21	0.02	27,31,34,36	16
5	SGN	C	6	19/20	0.20	-0.27	34,41,50,51	19
5	SGN	C	4	19/20	0.17	-0.94	32,35,39,40	19

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	SGN	A	3	19/20	0.38	2.49	55,60,70,70	19
3	EPE	D	211	15/15	0.22	0.97	6,16,23,24	0
3	EPE	B	211	15/15	0.17	0.05	22,41,45,46	0
3	EPE	A	211	15/15	0.18	-0.32	14,32,34,34	0
3	EPE	C	211	15/15	0.16	-0.96	44,54,59,59	0
2	SO4	A	1	5/5	0.12	-1.22	22,22,27,28	0
2	SO4	B	2	5/5	0.14	-1.39	10,11,14,19	0
2	SO4	C	3	5/5	0.12	-2.20	49,49,51,52	0
2	SO4	D	4	5/5	0.10	-2.48	34,37,38,40	0

6.5 Other polymers

There are no such residues in this entry.