



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 06:22 AM GMT

PDB ID : 1GMO
Title : CRYSTAL STRUCTURES OF NK1-HEPARIN COMPLEXES REVEAL THE BASIS FOR NK1 ACTIVITY AND ENABLE ENGINEERING OF POTENT AGONISTS OF THE MET RECEPTOR
Authors : Lietha, D.; Chirgadze, D.Y.; Mulloy, B.; Blundell, T.L.; Gherardi, E.
Deposited on : 2001-09-20
Resolution : 3.00 Å(reported)

This is a wwPDB validation summary 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>

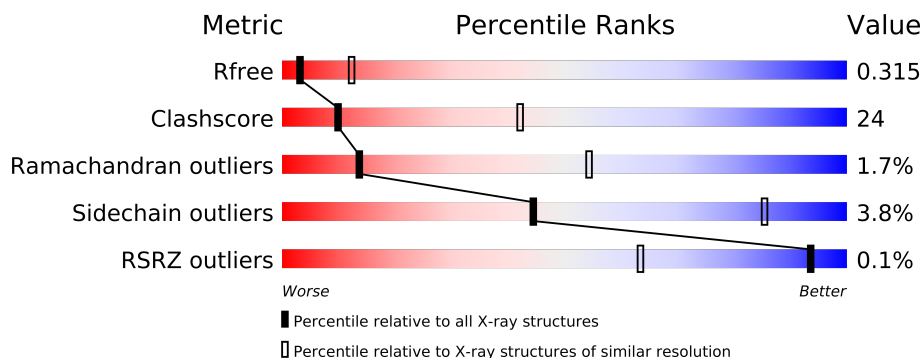
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.00 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	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)

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	
1	E	183	
1	F	183	
1	G	183	
1	H	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
3	SO4	A	1215	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
4	EPE	F	1218	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 11555 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	172	Total	C	N	O	S	0	0	0
			1324	833	228	251	12			
1	B	172	Total	C	N	O	S	0	0	0
			1339	843	231	253	12			
1	C	172	Total	C	N	O	S	0	0	0
			1341	846	231	252	12			
1	D	172	Total	C	N	O	S	0	0	0
			1305	821	223	249	12			
1	E	173	Total	C	N	O	S	0	0	0
			1297	812	222	251	12			
1	F	173	Total	C	N	O	S	0	0	0
			1331	836	231	252	12			
1	G	164	Total	C	N	O	S	0	0	0
			1241	783	212	234	12			
1	H	171	Total	C	N	O	S	0	0	0
			1299	814	224	249	12			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	29	VAL	ALA	ENGINEERED MUTATION	UNP P14210
A	72	ASP	ASN	ENGINEERED MUTATION	UNP P14210
B	29	VAL	ALA	ENGINEERED MUTATION	UNP P14210
B	72	ASP	ASN	ENGINEERED MUTATION	UNP P14210
C	29	VAL	ALA	ENGINEERED MUTATION	UNP P14210
C	72	ASP	ASN	ENGINEERED MUTATION	UNP P14210
D	29	VAL	ALA	ENGINEERED MUTATION	UNP P14210
D	72	ASP	ASN	ENGINEERED MUTATION	UNP P14210
E	29	VAL	ALA	ENGINEERED MUTATION	UNP P14210
E	72	ASP	ASN	ENGINEERED MUTATION	UNP P14210
F	29	VAL	ALA	ENGINEERED MUTATION	UNP P14210
F	72	ASP	ASN	ENGINEERED MUTATION	UNP P14210
G	29	VAL	ALA	ENGINEERED MUTATION	UNP P14210

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Chain	Residue	Modelled	Actual	Comment	Reference
G	72	ASP	ASN	ENGINEERED MUTATION	UNP P14210
H	29	VAL	ALA	ENGINEERED MUTATION	UNP P14210
H	72	ASP	ASN	ENGINEERED MUTATION	UNP P14210

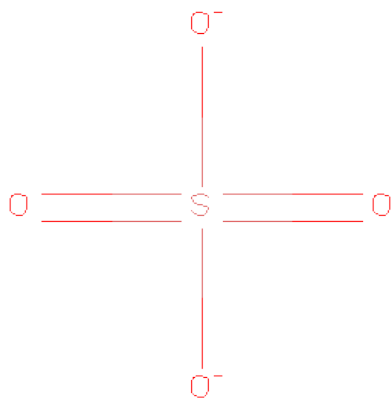
- Molecule 2 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	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
A	29	VAL	ALA	ENGINEERED MUTATION	UNP P14210
A	72	ASP	ASN	ENGINEERED MUTATION	UNP P14210

- Molecule 3 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



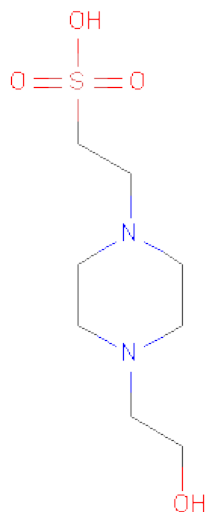
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		

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

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



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	G	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	H	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 5 is a polymer of unknown type called SUGAR (7-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	7	Total	C	N	O	S	0	0
			121	42	3	66	10		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	29	VAL	ALA	ENGINEERED MUTATION	UNP P14210
B	72	ASP	ASN	ENGINEERED MUTATION	UNP P14210

- Molecule 6 is a polymer of unknown type called SUGAR (8-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	8	Total	C	N	O	S	0	0
			140	48	4	76	12		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	29	VAL	ALA	ENGINEERED MUTATION	UNP P14210
B	72	ASP	ASN	ENGINEERED MUTATION	UNP P14210

- Molecule 7 is a polymer of unknown type called SUGAR (9-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	C	9	Total	C	N	O	S	0	0
			159	54	5	86	14		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	29	VAL	ALA	ENGINEERED MUTATION	UNP P14210
C	72	ASP	ASN	ENGINEERED MUTATION	UNP P14210

- Molecule 8 is a polymer of unknown type called SUGAR (6-MER).

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

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	29	VAL	ALA	ENGINEERED MUTATION	UNP P14210
F	72	ASP	ASN	ENGINEERED MUTATION	UNP P14210
G	29	VAL	ALA	ENGINEERED MUTATION	UNP P14210
G	72	ASP	ASN	ENGINEERED MUTATION	UNP P14210

- Molecule 9 is water.

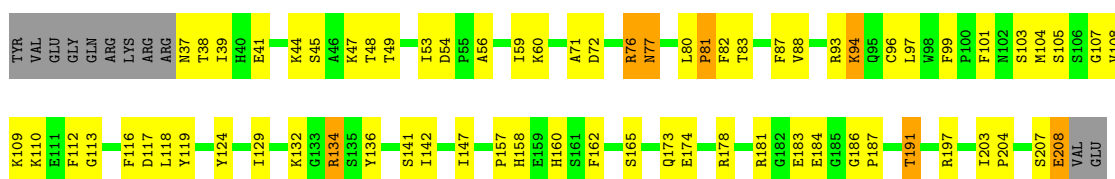
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	21	Total	O	0	0
			21	21		
9	B	34	Total	O	0	0
			34	34		
9	C	27	Total	O	0	0
			27	27		
9	D	22	Total	O	0	0
			22	22		
9	E	29	Total	O	0	0
			29	29		
9	F	20	Total	O	0	0
			20	20		
9	G	17	Total	O	0	0
			17	17		
9	H	13	Total	O	0	0
			13	13		

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.

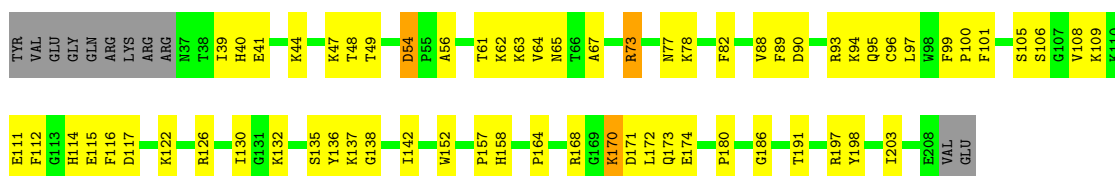
• Molecule 1: HEPATOCYTE GROWTH FACTOR

Chain A:



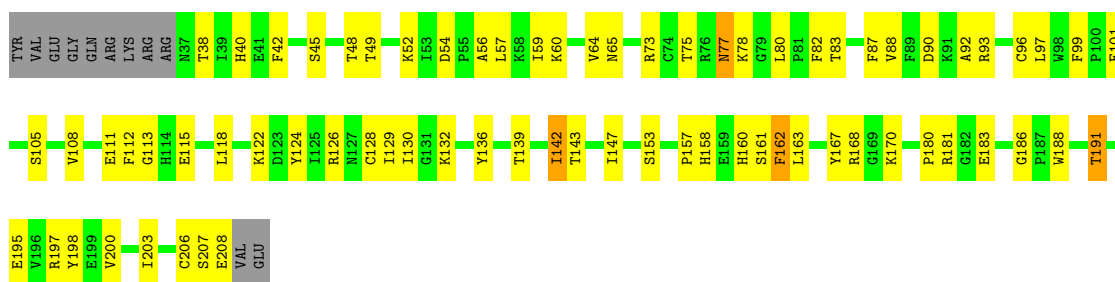
• Molecule 1: HEPATOCYTE GROWTH FACTOR

Chain B:



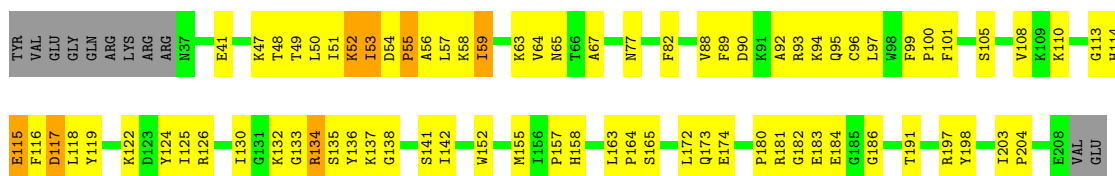
• Molecule 1: HEPATOCYTE GROWTH FACTOR

Chain C:



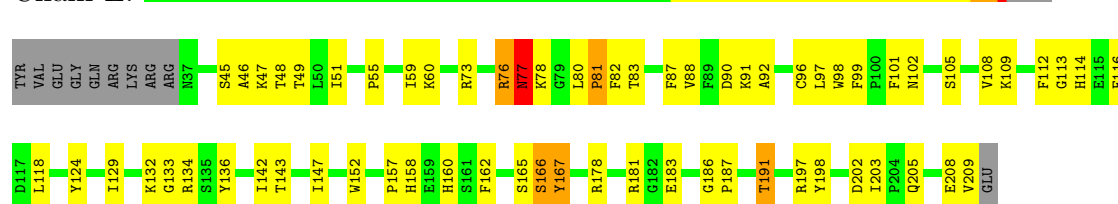
• Molecule 1: HEPATOCYTE GROWTH FACTOR

Chain D:



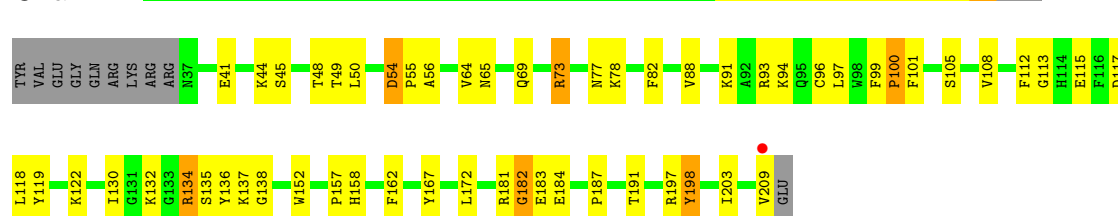
- Molecule 1: HEPATOCYTE GROWTH FACTOR

Chain E:



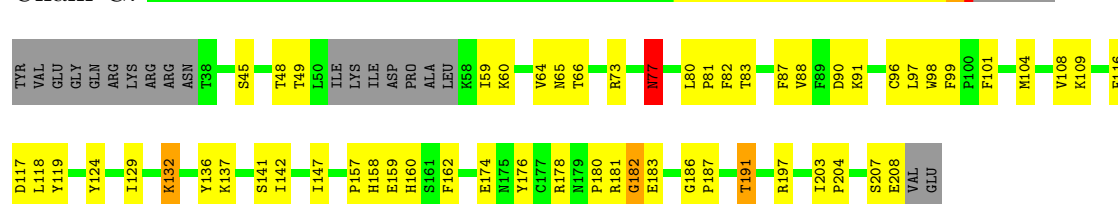
- Molecule 1: HEPATOCYTE GROWTH FACTOR

Chain F:



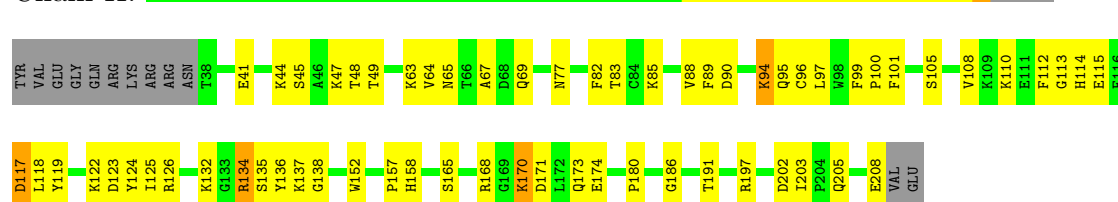
- Molecule 1: HEPATOCYTE GROWTH FACTOR

Chain G:



- Molecule 1: HEPATOCYTE GROWTH FACTOR

Chain H:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	179.70Å 174.10Å 59.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 19.97 – 2.97	Depositor EDS
% Data completeness (in resolution range)	95.3 (20.00-3.00) 94.6 (19.97-2.97)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.26 (at 2.98Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.254 , 0.295 0.272 , 0.315	Depositor DCC
R_{free} test set	1824 reflections (4.98%)	DCC
Wilson B-factor (Å ²)	59.5	Xtriage
Anisotropy	0.123	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 29.1	EDS
Estimated twinning fraction	0.005 for k,h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 37652 reflections	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	11555	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% 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	0.45	0/1358	0.67	0/1835
1	B	0.44	0/1374	0.63	0/1855
1	C	0.50	0/1376	0.67	0/1859
1	D	0.45	0/1338	0.63	0/1813
1	E	0.45	0/1331	0.66	0/1808
1	F	0.45	0/1365	0.66	0/1848
1	G	0.38	0/1273	0.62	0/1724
1	H	0.39	0/1334	0.59	0/1808
All	All	0.44	0/10749	0.64	0/14550

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	A	1	0
6	B	1	0
All	All	2	0

There are no bond length outliers.

There are no bond angle outliers.

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1213	IDS	C4
6	B	1223	IDS	C4

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	1324	0	1221	73	0
1	B	1339	0	1248	62	0
1	C	1341	0	1257	71	0
1	D	1305	0	1193	73	0
1	E	1297	0	1140	72	0
1	F	1331	0	1223	56	0
1	G	1241	0	1121	55	0
1	H	1299	0	1162	55	0
2	A	105	0	39	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	2	0
3	D	5	0	0	1	0
3	E	5	0	0	0	0
3	F	10	0	0	2	0
3	H	5	0	0	1	0
4	A	15	0	17	1	0
4	B	15	0	17	2	0
4	C	15	0	17	3	0
4	D	15	0	17	1	0
4	E	15	0	17	1	0
4	F	15	0	17	1	0
4	G	15	0	17	0	0
4	H	15	0	17	0	0
5	B	121	0	44	1	0
6	B	140	0	52	3	0
7	C	159	0	61	2	0
8	F	105	0	40	1	0
8	G	105	0	40	0	0
9	A	21	0	0	0	0
9	B	34	0	0	5	0
9	C	27	0	0	6	0
9	D	22	0	0	7	0
9	E	29	0	0	7	0
9	F	20	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	G	17	0	0	3	0
9	H	13	0	0	1	0
All	All	11555	0	9977	513	0

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 24.

The worst 5 of 513 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:181:ARG:NH2	1:H:165:SER:HB3	1.63	1.12
1:D:52:LYS:H	1:D:52:LYS:HD3	1.22	1.01
1:A:134:ARG:HD2	1:A:134:ARG:H	1.26	0.98
1:F:64:VAL:HG13	1:F:69:GLN:OE1	1.64	0.96
1:G:132:LYS:H	1:G:132:LYS:HD2	1.31	0.96

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	170/183 (93%)	152 (89%)	15 (9%)	3 (2%)	13	53
1	B	170/183 (93%)	152 (89%)	17 (10%)	1 (1%)	33	81
1	C	170/183 (93%)	147 (86%)	22 (13%)	1 (1%)	33	81
1	D	170/183 (93%)	148 (87%)	18 (11%)	4 (2%)	9	42
1	E	171/183 (93%)	148 (86%)	18 (10%)	5 (3%)	7	35
1	F	171/183 (93%)	149 (87%)	18 (10%)	4 (2%)	10	43
1	G	160/183 (87%)	142 (89%)	14 (9%)	4 (2%)	9	40
1	H	169/183 (92%)	147 (87%)	21 (12%)	1 (1%)	33	81
All	All	1351/1464 (92%)	1185 (88%)	143 (11%)	23 (2%)	14	54

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	THR
1	E	77	ASN
1	E	91	LYS
1	F	55	PRO
1	F	182	GLY

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	140/165 (85%)	133 (95%)	7 (5%)	34	77
1	B	144/165 (87%)	140 (97%)	4 (3%)	56	91
1	C	145/165 (88%)	141 (97%)	4 (3%)	56	91
1	D	137/165 (83%)	130 (95%)	7 (5%)	33	76
1	E	132/165 (80%)	129 (98%)	3 (2%)	63	93
1	F	141/165 (86%)	135 (96%)	6 (4%)	40	82
1	G	129/165 (78%)	125 (97%)	4 (3%)	52	89
1	H	135/165 (82%)	128 (95%)	7 (5%)	32	75
All	All	1103/1320 (84%)	1061 (96%)	42 (4%)	44	85

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	117	ASP
1	E	77	ASN
1	H	134	ARG
1	D	134	ARG
1	D	191	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	158	HIS
1	E	160	HIS
1	G	65	ASN

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Mol	Chain	Res	Type
1	D	65	ASN
1	G	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 ⓘ

42 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
2	IDS	A	1209	2	17,17,17	1.30	3 (17%)	26,26,26	1.69	4 (15%)
2	SGN	A	1210	2	17,19,20	1.25	2 (11%)	24,29,31	2.30	4 (16%)
2	IDS	A	1211	2	15,16,17	1.39	3 (20%)	20,24,26	2.66	7 (35%)
2	SGN	A	1212	2	17,19,20	1.52	2 (11%)	24,29,31	2.40	4 (16%)
2	IDS	A	1213	2	15,16,17	1.29	3 (20%)	20,24,26	3.81	4 (20%)
2	SGN	A	1214	2	16,18,20	1.50	1 (6%)	18,27,31	2.48	4 (22%)
5	IDS	B	1209	5	17,17,17	1.62	4 (23%)	26,26,26	2.55	7 (26%)
5	SGN	B	1210	5	17,19,20	1.33	1 (5%)	24,29,31	2.20	4 (16%)
5	IDS	B	1211	5	15,16,17	1.26	2 (13%)	20,24,26	2.08	5 (25%)
5	SGN	B	1212	5	17,19,20	1.16	1 (5%)	24,29,31	2.46	5 (20%)
5	IDS	B	1213	5	15,16,17	1.34	2 (13%)	20,24,26	1.97	7 (35%)
5	SGN	B	1214	5	17,19,20	1.42	1 (5%)	24,29,31	2.30	5 (20%)
5	IDS	B	1215	5	14,15,17	1.12	1 (7%)	14,22,26	2.26	3 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	IDS	B	1217	6	17,17,17	1.64	3 (17%)	26,26,26	2.58	7 (26%)
6	SGN	B	1218	6	17,19,20	1.35	1 (5%)	24,29,31	2.51	4 (16%)
6	IDS	B	1219	6	15,16,17	1.23	2 (13%)	20,24,26	1.45	3 (15%)
6	SGN	B	1220	6	17,19,20	0.94	1 (5%)	24,29,31	2.04	5 (20%)
6	IDS	B	1221	6	15,16,17	1.30	2 (13%)	20,24,26	2.60	7 (35%)
6	SGN	B	1222	6	17,19,20	1.43	2 (11%)	24,29,31	2.50	4 (16%)
6	IDS	B	1223	6	15,16,17	1.44	3 (20%)	20,24,26	3.87	5 (25%)
6	SGN	B	1224	6	16,18,20	1.51	1 (6%)	18,27,31	2.26	3 (16%)
7	SGN	C	1210	7	20,20,20	1.58	4 (20%)	30,31,31	2.76	10 (33%)
7	IDS	C	1211	7	15,16,17	1.30	2 (13%)	20,24,26	2.20	6 (30%)
7	SGN	C	1212	7	17,19,20	1.35	2 (11%)	24,29,31	2.44	5 (20%)
7	IDS	C	1213	7	15,16,17	1.10	2 (13%)	20,24,26	1.89	5 (25%)
7	SGN	C	1214	7	17,19,20	0.89	0	24,29,31	1.88	4 (16%)
7	IDS	C	1215	7	15,16,17	1.18	2 (13%)	20,24,26	1.61	5 (25%)
7	SGN	C	1216	7	17,19,20	1.19	1 (5%)	24,29,31	2.38	8 (33%)
7	IDS	C	1217	7	15,16,17	1.25	2 (13%)	20,24,26	1.65	5 (25%)
7	SGN	C	1218	7	16,18,20	1.43	2 (12%)	18,27,31	2.32	4 (22%)
8	SGN	F	1210	8	20,20,20	1.63	3 (15%)	30,31,31	2.21	5 (16%)
8	IDS	F	1211	8	15,16,17	1.23	2 (13%)	20,24,26	1.90	7 (35%)
8	SGN	F	1212	8	17,19,20	1.27	1 (5%)	24,29,31	2.41	5 (20%)
8	IDS	F	1213	8	15,16,17	1.32	4 (26%)	20,24,26	2.12	6 (30%)
8	SGN	F	1214	8	17,19,20	1.38	1 (5%)	24,29,31	2.45	5 (20%)
8	IDS	F	1215	8	14,15,17	0.96	1 (7%)	14,22,26	2.55	3 (21%)
8	SGN	G	1209	8	20,20,20	1.51	3 (15%)	30,31,31	2.91	5 (16%)
8	IDS	G	1210	8	15,16,17	1.29	2 (13%)	20,24,26	1.60	4 (20%)
8	SGN	G	1211	8	17,19,20	1.37	1 (5%)	24,29,31	2.54	5 (20%)
8	IDS	G	1212	8	15,16,17	1.37	3 (20%)	20,24,26	2.67	6 (30%)
8	SGN	G	1213	8	17,19,20	1.76	3 (17%)	24,29,31	2.39	5 (20%)
8	IDS	G	1214	8	14,15,17	0.91	1 (7%)	14,22,26	2.67	3 (21%)

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	IDS	A	1209	2	-	0/9/29/29	0/1/1/1
2	SGN	A	1210	2	-	0/11/28/31	0/1/1/1
2	IDS	A	1211	2	-	0/9/26/29	0/1/1/1
2	SGN	A	1212	2	-	0/11/28/31	0/1/1/1
2	IDS	A	1213	2	1/1/6/7	1/9/26/29	0/1/1/1
2	SGN	A	1214	2	-	0/11/24/31	0/1/1/1
5	IDS	B	1209	5	-	0/9/29/29	0/1/1/1
5	SGN	B	1210	5	-	0/11/28/31	0/1/1/1
5	IDS	B	1211	5	-	0/9/26/29	0/1/1/1
5	SGN	B	1212	5	-	0/11/28/31	0/1/1/1
5	IDS	B	1213	5	-	0/9/26/29	0/1/1/1
5	SGN	B	1214	5	-	0/11/28/31	0/1/1/1
5	IDS	B	1215	5	-	0/9/22/29	0/1/1/1
6	IDS	B	1217	6	-	1/9/29/29	0/1/1/1
6	SGN	B	1218	6	-	0/11/28/31	0/1/1/1
6	IDS	B	1219	6	-	0/9/26/29	0/1/1/1
6	SGN	B	1220	6	-	0/11/28/31	0/1/1/1
6	IDS	B	1221	6	-	0/9/26/29	0/1/1/1
6	SGN	B	1222	6	-	0/11/28/31	0/1/1/1
6	IDS	B	1223	6	1/1/6/7	1/9/26/29	0/1/1/1
6	SGN	B	1224	6	-	0/11/24/31	0/1/1/1
7	SGN	C	1210	7	-	0/11/31/31	0/1/1/1
7	IDS	C	1211	7	-	0/9/26/29	0/1/1/1
7	SGN	C	1212	7	-	0/11/28/31	0/1/1/1
7	IDS	C	1213	7	-	0/9/26/29	0/1/1/1
7	SGN	C	1214	7	-	0/11/28/31	0/1/1/1
7	IDS	C	1215	7	-	0/9/26/29	0/1/1/1
7	SGN	C	1216	7	-	0/11/28/31	0/1/1/1
7	IDS	C	1217	7	-	0/9/26/29	0/1/1/1
7	SGN	C	1218	7	-	0/11/24/31	0/1/1/1
8	SGN	F	1210	8	-	0/11/31/31	0/1/1/1
8	IDS	F	1211	8	-	0/9/26/29	0/1/1/1
8	SGN	F	1212	8	-	0/11/28/31	0/1/1/1
8	IDS	F	1213	8	-	0/9/26/29	0/1/1/1
8	SGN	F	1214	8	-	0/11/28/31	0/1/1/1
8	IDS	F	1215	8	-	1/9/22/29	0/1/1/1
8	SGN	G	1209	8	-	0/11/31/31	0/1/1/1
8	IDS	G	1210	8	-	0/9/26/29	0/1/1/1
8	SGN	G	1211	8	-	0/11/28/31	0/1/1/1
8	IDS	G	1212	8	-	0/9/26/29	0/1/1/1
8	SGN	G	1213	8	-	0/11/28/31	0/1/1/1
8	IDS	G	1214	8	-	1/9/22/29	0/1/1/1

The worst 5 of 83 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	G	1213	SGN	S1-N	5.58	1.66	1.60
8	F	1210	SGN	S1-N	5.18	1.65	1.60
2	A	1214	SGN	S1-N	4.83	1.65	1.60
2	A	1212	SGN	S1-N	4.83	1.65	1.60
6	B	1224	SGN	S1-N	4.58	1.65	1.60

The worst 5 of 212 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1223	IDS	O4-C4-C3	14.92	143.81	110.35
2	A	1213	IDS	O4-C4-C3	14.55	142.99	110.35
8	G	1209	SGN	O4-C4-C3	-11.42	84.74	110.35
6	B	1218	SGN	C6-O6-S2	10.53	130.30	116.76
7	C	1210	SGN	O4-C4-C3	-10.29	87.27	110.35

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	B	1223	IDS	C4
2	A	1213	IDS	C4

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1213	IDS	S-O2-C2-C1
8	G	1214	IDS	S-O2-C2-C1
8	F	1215	IDS	S-O2-C2-C1
6	B	1223	IDS	S-O2-C2-C1
6	B	1217	IDS	S-O2-C2-C1

There are no ring outliers.

5.6 Ligand geometry ⓘ

16 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	A	1215	-	4,4,4	3.43	2 (50%)	6,6,6	0.94	0
4	EPE	A	1216	-	15,15,15	1.09	1 (6%)	20,20,20	0.99	1 (5%)
3	SO4	B	1216	-	4,4,4	3.44	2 (50%)	6,6,6	0.93	0
4	EPE	B	1225	-	15,15,15	1.33	3 (20%)	20,20,20	1.08	2 (10%)
3	SO4	C	1209	-	4,4,4	3.05	2 (50%)	6,6,6	1.03	0
4	EPE	C	1219	-	15,15,15	0.94	0	20,20,20	1.08	2 (10%)
3	SO4	D	1209	-	4,4,4	3.59	2 (50%)	6,6,6	0.92	0
4	EPE	D	1210	-	15,15,15	1.19	2 (13%)	20,20,20	0.92	0
3	SO4	E	1210	-	4,4,4	3.42	2 (50%)	6,6,6	1.02	0
4	EPE	E	1211	-	15,15,15	1.06	1 (6%)	20,20,20	1.13	3 (15%)
3	SO4	F	1216	-	4,4,4	3.49	2 (50%)	6,6,6	0.92	0
3	SO4	F	1217	-	4,4,4	3.48	2 (50%)	6,6,6	0.92	0
4	EPE	F	1218	-	15,15,15	1.40	3 (20%)	20,20,20	0.78	0
4	EPE	G	1215	-	15,15,15	1.21	1 (6%)	20,20,20	0.90	0
3	SO4	H	1209	-	4,4,4	3.49	2 (50%)	6,6,6	0.94	0
4	EPE	H	1210	-	15,15,15	1.08	1 (6%)	20,20,20	0.97	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
3	SO4	A	1215	-	-	0/0/0/0	0/0/0/0
4	EPE	A	1216	-	-	0/9/19/19	0/1/1/1
3	SO4	B	1216	-	-	0/0/0/0	0/0/0/0
4	EPE	B	1225	-	-	0/9/19/19	0/1/1/1
3	SO4	C	1209	-	-	0/0/0/0	0/0/0/0
4	EPE	C	1219	-	-	0/9/19/19	0/1/1/1
3	SO4	D	1209	-	-	0/0/0/0	0/0/0/0
4	EPE	D	1210	-	-	0/9/19/19	0/1/1/1
3	SO4	E	1210	-	-	0/0/0/0	0/0/0/0
4	EPE	E	1211	-	-	0/9/19/19	0/1/1/1
3	SO4	F	1216	-	-	0/0/0/0	0/0/0/0
3	SO4	F	1217	-	-	0/0/0/0	0/0/0/0
4	EPE	F	1218	-	-	0/9/19/19	0/1/1/1
4	EPE	G	1215	-	-	0/9/19/19	0/1/1/1
3	SO4	H	1209	-	-	0/0/0/0	0/0/0/0
4	EPE	H	1210	-	-	0/9/19/19	0/1/1/1

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1209	SO4	O3-S	-5.03	1.30	1.47
3	H	1209	SO4	O3-S	-5.00	1.30	1.47
3	E	1210	SO4	O1-S	4.99	1.63	1.47
3	F	1216	SO4	O1-S	4.97	1.63	1.47
3	F	1217	SO4	O1-S	4.94	1.63	1.47

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1225	EPE	O1S-S-C10	-2.67	104.52	106.81
4	H	1210	EPE	O1S-S-C10	-2.57	104.60	106.81
4	B	1225	EPE	O2S-S-C10	2.46	108.92	106.81
4	C	1219	EPE	O1S-S-C10	-2.15	104.96	106.81
4	E	1211	EPE	O1S-S-C10	-2.12	104.99	106.81

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	172/183 (93%)	-0.03	0	100 100	22, 50, 91, 102	0
1	B	172/183 (93%)	-0.20	0	100 100	18, 47, 84, 94	0
1	C	172/183 (93%)	-0.28	0	100 100	10, 35, 55, 72	0
1	D	172/183 (93%)	-0.14	0	100 100	17, 48, 87, 90	0
1	E	173/183 (94%)	-0.09	0	100 100	22, 54, 88, 98	0
1	F	173/183 (94%)	-0.13	1 (0%)	86 32	18, 49, 92, 109	0
1	G	164/183 (89%)	0.11	0	100 100	43, 69, 95, 103	0
1	H	171/183 (93%)	0.08	0	100 100	24, 65, 114, 129	0
All	All	1369/1464 (93%)	-0.09	1 (0%)	93 63	10, 52, 94, 129	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	209	VAL	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(\AA^2)	Q<0.9
5	IDS	B	1213	16/17	0.45	18.67	139,140,141,144	0
5	SGN	B	1214	19/20	0.44	13.81	143,145,146,147	0
8	IDS	F	1213	16/17	0.29	10.21	134,135,136,137	0
6	IDS	B	1217	17/17	0.34	6.26	106,114,118,118	0
5	IDS	B	1211	16/17	0.41	5.68	138,140,142,142	0
8	IDS	G	1210	16/17	0.36	5.13	122,129,131,131	0
8	SGN	F	1210	20/20	0.51	4.68	143,150,155,155	0
5	SGN	B	1210	19/20	0.42	4.63	138,141,143,143	0
5	IDS	B	1209	17/17	0.46	3.90	142,145,146,146	0
8	SGN	G	1209	20/20	0.47	3.63	131,137,140,140	0
8	SGN	F	1214	19/20	0.37	3.22	132,135,137,137	0
7	SGN	C	1212	19/20	0.30	3.20	94,101,106,106	0
2	IDS	A	1209	17/17	0.45	3.08	121,122,123,123	0
5	IDS	B	1215	15/17	0.52	2.37	144,144,145,145	0
2	SGN	A	1210	19/20	0.32	2.02	120,121,124,124	0
8	IDS	G	1214	15/17	0.43	2.00	125,125,126,127	0
7	SGN	C	1218	18/20	0.34	1.68	118,126,130,130	0
2	SGN	A	1214	18/20	0.43	1.40	132,134,142,142	0
6	SGN	B	1224	18/20	0.30	1.12	124,127,129,129	0
8	IDS	F	1215	15/17	0.31	0.96	127,130,132,132	0
2	SGN	A	1212	19/20	0.43	0.89	123,125,127,127	0
8	SGN	G	1213	19/20	0.39	0.74	125,126,129,129	0
2	IDS	A	1213	16/17	0.36	0.68	125,127,130,131	0
6	SGN	B	1218	19/20	0.22	0.63	95,103,105,105	0
7	SGN	C	1210	20/20	0.22	0.47	105,112,122,122	0
8	IDS	G	1212	16/17	0.30	0.27	123,124,126,127	0
6	IDS	B	1223	16/17	0.28	0.14	106,112,115,123	0
2	IDS	A	1211	16/17	0.28	-0.11	118,121,122,122	0
6	SGN	B	1222	19/20	0.19	-0.60	97,103,107,109	0
5	SGN	B	1212	19/20	0.26	-0.73	134,137,138,138	0
7	SGN	C	1214	19/20	0.19	-0.81	55,60,67,74	0
7	SGN	C	1216	19/20	0.17	-0.81	75,79,81,89	0
7	IDS	C	1213	16/17	0.18	-0.83	71,87,89,91	0
6	SGN	B	1220	19/20	0.20	-0.92	70,79,82,89	0
6	IDS	B	1221	16/17	0.17	-1.05	93,97,102,102	0
8	SGN	G	1211	19/20	0.20	-1.22	119,120,121,122	0
7	IDS	C	1217	16/17	0.18	-1.36	90,95,101,114	0
7	IDS	C	1215	16/17	0.13	-1.67	76,78,82,82	0
8	SGN	F	1212	19/20	0.23	-1.77	127,131,132,133	0
6	IDS	B	1219	16/17	0.24	-	82,90,92,93	0
8	IDS	F	1211	16/17	0.43	-	134,140,143,143	0
7	IDS	C	1211	16/17	0.26	-	103,106,106,106	0

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
3	SO4	A	1215	5/5	0.32	6.10	126,126,127,127	0
4	EPE	F	1218	15/15	0.42	5.42	102,103,104,105	0
4	EPE	C	1219	15/15	0.26	1.59	46,50,53,53	0
3	SO4	F	1217	5/5	0.24	1.33	133,133,133,134	0
4	EPE	G	1215	15/15	0.29	0.99	73,80,86,86	0
4	EPE	A	1216	15/15	0.20	0.86	35,37,43,44	0
4	EPE	E	1211	15/15	0.22	0.80	64,69,70,70	0
3	SO4	C	1209	5/5	0.19	0.30	108,108,109,110	0
4	EPE	D	1210	15/15	0.19	0.09	62,67,68,68	0
3	SO4	D	1209	5/5	0.20	0.02	102,102,102,103	0
4	EPE	B	1225	15/15	0.19	-0.21	35,46,53,53	0
3	SO4	E	1210	5/5	0.16	-0.42	94,94,95,95	0
3	SO4	F	1216	5/5	0.17	-0.44	111,112,112,112	0
3	SO4	B	1216	5/5	0.14	-0.72	101,101,101,101	0
3	SO4	H	1209	5/5	0.13	-0.73	82,83,83,83	0
4	EPE	H	1210	15/15	0.15	-1.09	54,55,57,58	0

6.5 Other polymers ⓘ

There are no such residues in this entry.