



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:02 AM UTC

PDB ID : 5SX5 / pdb_00005sx5
Title : Crystal Structure of panitumumab in complex with epidermal growth factor receptor domain 3 mutant S468R.
Authors : Sickmier, E.A.
Deposited on : 2016-08-09
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

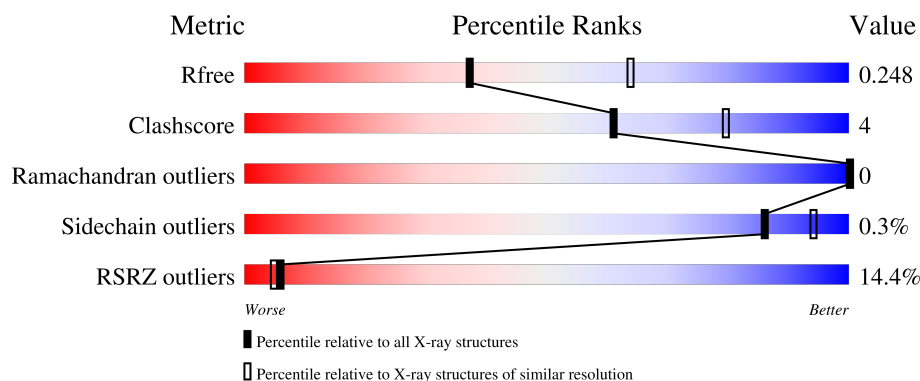
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	K	214	3% 89% 10%
1	L	214	% 89% 10% .
2	H	221	5% 88% 5% 6%
2	J	221	8% 79% 14% 6%
3	M	201	39% 87% 9% .

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Mol	Chain	Length	Quality of chain
3	N	201	31% 83% 13%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 9644 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Panitumumab Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	K	213	Total	C	N	O	S	0	0	0
			1637	1025	273	334	5			
1	L	212	Total	C	N	O	S	0	0	0
			1628	1020	272	331	5			

- Molecule 2 is a protein called Panitumumab Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	J	207	Total	C	N	O	S	0	0	0
			1556	985	254	311	6			
2	H	207	Total	C	N	O	S	0	0	0
			1556	985	254	311	6			

- Molecule 3 is a protein called Epidermal growth factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	194	Total	C	N	O	S	0	0	0
			1502	943	269	282	8			
3	N	192	Total	C	N	O	S	0	0	0
			1482	931	263	280	8			

There are 26 discrepancies between the modelled and reference sequences:

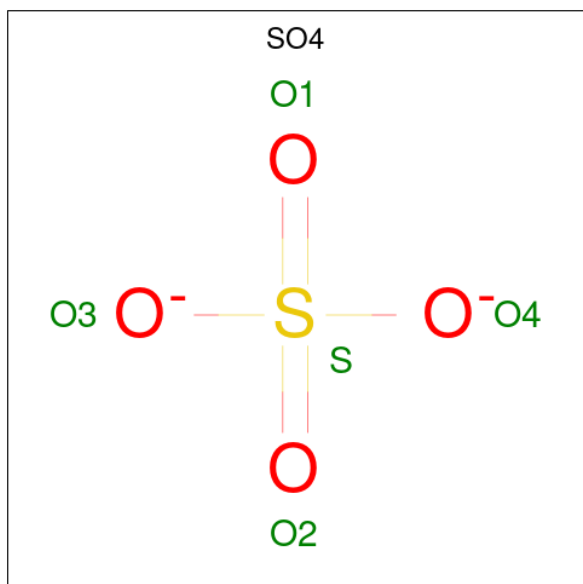
Chain	Residue	Modelled	Actual	Comment	Reference
M	307	LEU	-	expression tag	UNP P00533
M	308	GLU	-	expression tag	UNP P00533
M	309	GLU	-	expression tag	UNP P00533
M	310	LYS	-	expression tag	UNP P00533
M	328	ASP	ASN	conflict	UNP P00533
M	420	ASP	ASN	conflict	UNP P00533
M	468	ARG	SER	engineered mutation	UNP P00533
M	1502	HIS	-	expression tag	UNP P00533

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Chain	Residue	Modelled	Actual	Comment	Reference
M	1503	HIS	-	expression tag	UNP P00533
M	1504	HIS	-	expression tag	UNP P00533
M	1505	HIS	-	expression tag	UNP P00533
M	1506	HIS	-	expression tag	UNP P00533
M	1507	HIS	-	expression tag	UNP P00533
N	307	LEU	-	expression tag	UNP P00533
N	308	GLU	-	expression tag	UNP P00533
N	309	GLU	-	expression tag	UNP P00533
N	310	LYS	-	expression tag	UNP P00533
N	328	ASP	ASN	conflict	UNP P00533
N	420	ASP	ASN	conflict	UNP P00533
N	468	ARG	SER	engineered mutation	UNP P00533
N	502	HIS	-	expression tag	UNP P00533
N	503	HIS	-	expression tag	UNP P00533
N	504	HIS	-	expression tag	UNP P00533
N	505	HIS	-	expression tag	UNP P00533
N	506	HIS	-	expression tag	UNP P00533
N	507	HIS	-	expression tag	UNP P00533

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



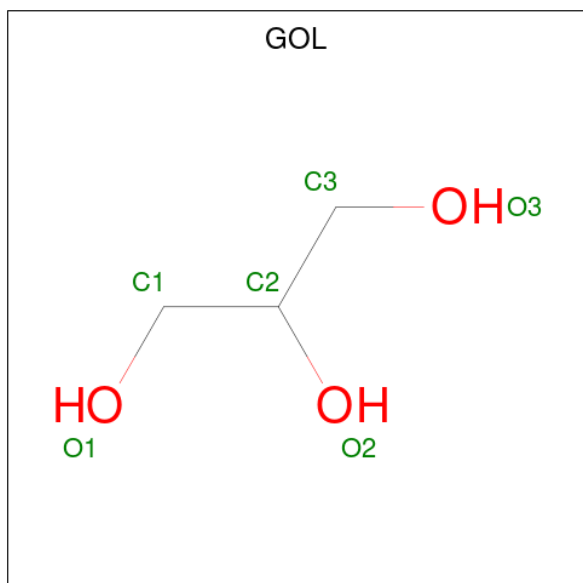
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	K	1	Total	O	S	0	0
			5	4	1		
4	K	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	K	1	Total	O	S	0	0
			5	4	1		
4	L	1	Total	O	S	0	0
			5	4	1		
4	L	1	Total	O	S	0	0
			5	4	1		
4	L	1	Total	O	S	0	0
			5	4	1		
4	L	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		
4	N	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



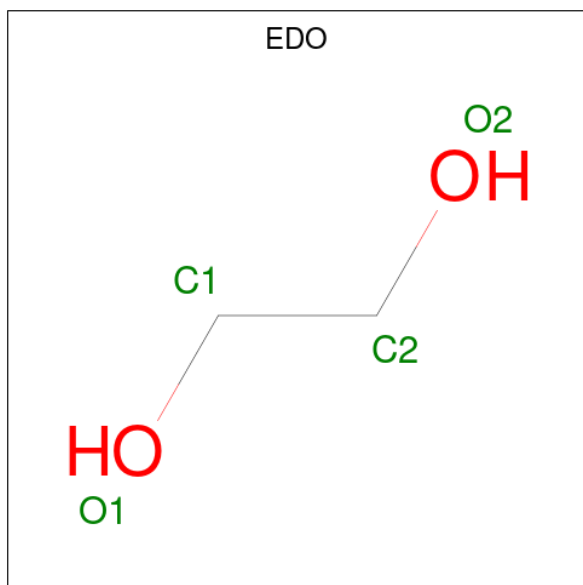
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	K	1	Total	C	O	0	0
			6	3	3		

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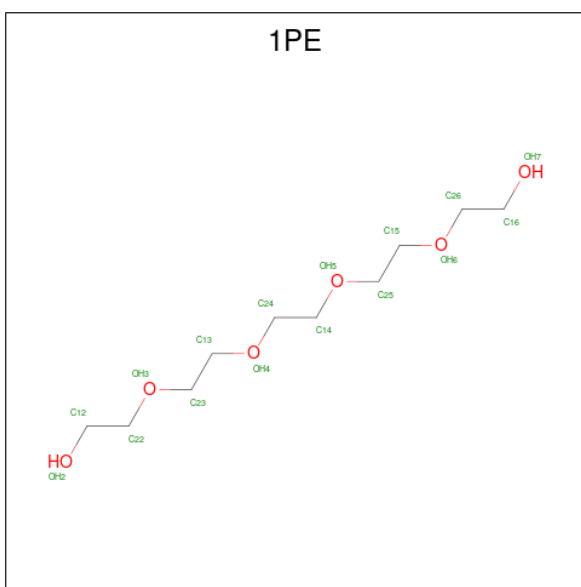
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	K	1	Total	C	O	0	0
			6	3	3		
5	L	1	Total	C	O	0	0
			6	3	3		
5	H	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	K	1	Total	C	O	0	0
			4	2	2		
6	J	1	Total	C	O	0	0
			4	2	2		
6	H	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	J	1	Total	C	O	0	0
			16	10	6		
7	L	1	Total	C	O	0	0
			16	10	6		
7	H	1	Total	C	O	0	0
			16	10	6		

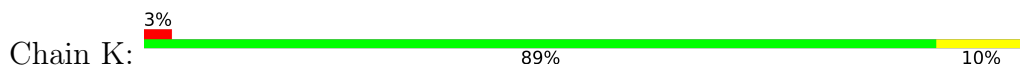
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	K	43	Total	O	0	0
			43	43		
8	J	21	Total	O	0	0
			21	21		
8	L	38	Total	O	0	0
			38	38		
8	H	30	Total	O	0	0
			30	30		
8	M	4	Total	O	0	0
			4	4		
8	N	3	Total	O	0	0
			3	3		

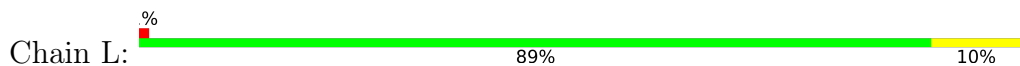
3 Residue-property plots [i](#)

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.

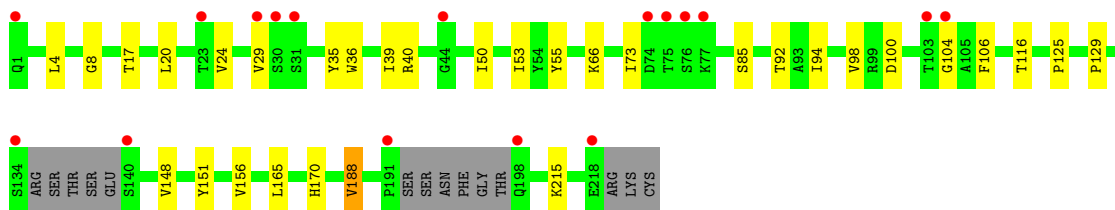
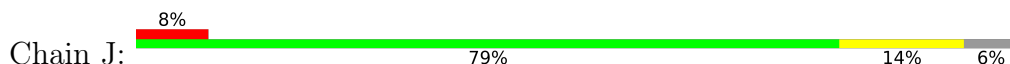
- Molecule 1: Panitumumab Fab Light Chain



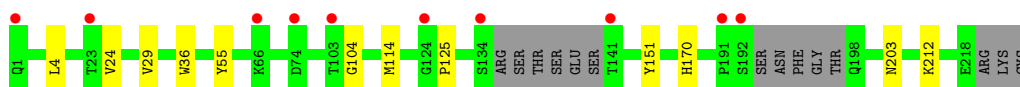
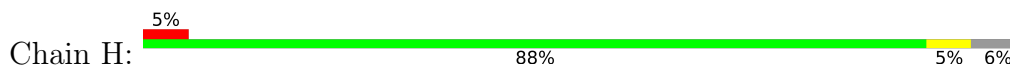
- Molecule 1: Panitumumab Fab Light Chain



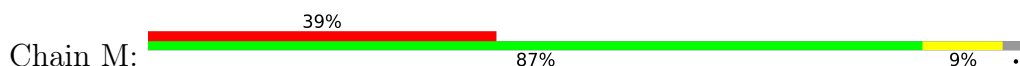
- Molecule 2: Panitumumab Fab Heavy Chain

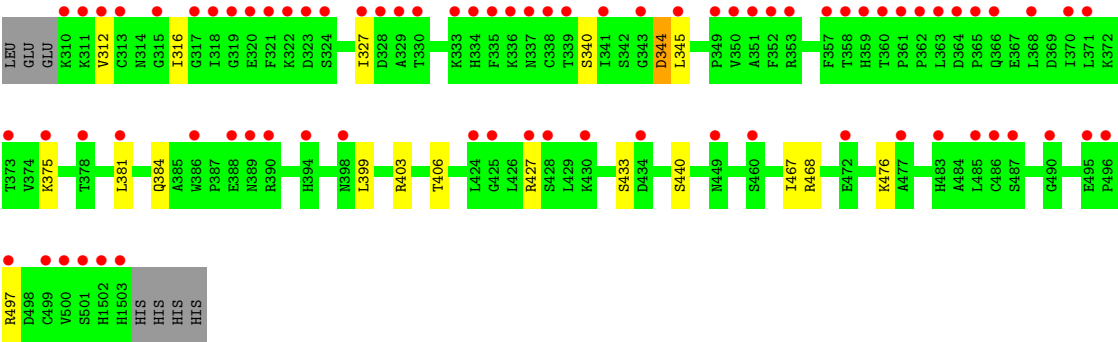


- Molecule 2: Panitumumab Fab Heavy Chain

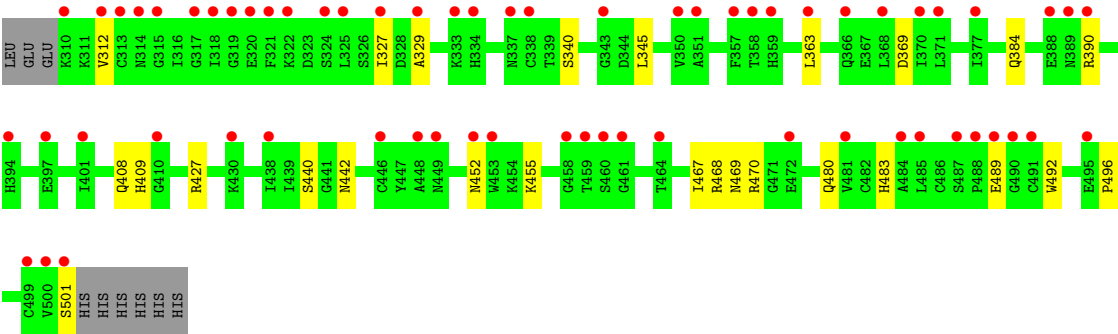
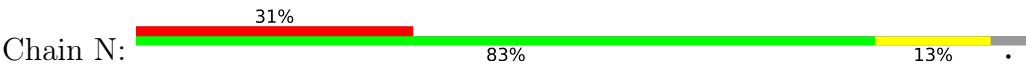


- Molecule 3: Epidermal growth factor receptor





• Molecule 3: Epidermal growth factor receptor



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.07Å 113.11Å 231.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.98 – 2.50 29.98 – 2.50	Depositor EDS
% Data completeness (in resolution range)	91.8 (29.98-2.50) 87.3 (29.98-2.50)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.92 (at 2.51Å)	Xtriage
Refinement program	PHENIX dev_2356	Depositor
R, R_{free}	0.226 , 0.250 0.227 , 0.248	Depositor DCC
R_{free} test set	2687 reflections (4.47%)	wwPDB-VP
Wilson B-factor (Å ²)	35.2	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 45.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9644	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 1PE, GOL, EDO, 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	K	0.09	0/1673	0.29	0/2272
1	L	0.09	0/1664	0.30	0/2260
2	H	0.10	0/1593	0.30	0/2177
2	J	0.09	0/1593	0.31	0/2177
3	M	0.09	0/1532	0.28	0/2070
3	N	0.08	0/1510	0.27	0/2040
All	All	0.09	0/9565	0.29	0/12996

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

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	K	1637	0	1579	15	0
1	L	1628	0	1573	13	0
2	H	1556	0	1525	9	0
2	J	1556	0	1523	21	0
3	M	1502	0	1498	13	0
3	N	1482	0	1482	18	0
4	H	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	K	15	0	0	1	0
4	L	25	0	0	1	0
4	N	5	0	0	0	0
5	H	6	0	8	0	0
5	K	12	0	16	1	0
5	L	6	0	8	0	0
6	H	4	0	6	0	0
6	J	4	0	6	0	0
6	K	4	0	6	0	0
7	H	16	0	22	1	0
7	J	16	0	22	2	0
7	L	16	0	22	0	0
8	H	30	0	0	0	0
8	J	21	0	0	0	0
8	K	43	0	0	1	0
8	L	38	0	0	0	0
8	M	4	0	0	0	0
8	N	3	0	0	0	0
All	All	9644	0	9296	78	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (78) 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)
3:N:327:ILE:HD11	3:N:345:LEU:HD22	1.71	0.71
1:K:91:PHE:HA	1:K:96:LEU:HD22	1.77	0.66
2:J:55:TYR:OH	3:M:384:GLN:NE2	2.30	0.64
3:M:375:LYS:HA	3:M:399:LEU:HA	1.78	0.64
3:N:452:ASN:HB3	3:N:455:LYS:HE3	1.81	0.62
2:J:94:ILE:HD11	7:J:301:1PE:H262	1.82	0.62
1:L:91:PHE:HA	1:L:96:LEU:HD22	1.82	0.61
1:K:9:SER:H	5:K:304:GOL:H2	1.66	0.60
2:H:125:PRO:HB3	2:H:151:TYR:HB3	1.83	0.60
3:N:442:ASN:H	3:N:469:ASN:HD22	1.50	0.60
2:J:94:ILE:HD13	7:J:301:1PE:H131	1.84	0.60
1:L:96:LEU:HD21	3:N:468:ARG:HG2	1.82	0.60
3:M:427:ARG:HH21	3:M:497:ARG:HB2	1.66	0.59
1:L:40:PRO:HB3	1:L:165:GLU:HG3	1.85	0.58
3:M:344:ASP:OD1	3:M:406:THR:OG1	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:4:LEU:HD22	2:J:24:VAL:HG22	1.85	0.57
2:H:104:GLY:HA2	3:N:468:ARG:HH22	1.69	0.56
1:L:120:PRO:HD3	1:L:132:VAL:HG22	1.87	0.56
1:K:120:PRO:HD3	1:K:132:VAL:HG22	1.88	0.55
1:K:93:HIS:NE2	4:K:303:SO4:O1	2.34	0.55
1:L:123:GLU:OE1	1:L:123:GLU:N	2.37	0.54
2:H:104:GLY:HA2	3:N:468:ARG:NH2	2.21	0.54
3:N:329:ALA:HB2	3:N:363:LEU:HA	1.90	0.54
2:H:4:LEU:HD22	2:H:24:VAL:HG22	1.89	0.53
2:J:125:PRO:HB3	2:J:151:TYR:HB3	1.91	0.53
1:K:96:LEU:HD21	3:M:468:ARG:HG2	1.90	0.53
1:K:45:LYS:NZ	8:K:404:HOH:O	2.42	0.52
2:J:104:GLY:HA2	3:M:468:ARG:NH2	2.24	0.52
2:J:53:ILE:HD13	2:J:73:ILE:HG13	1.91	0.52
1:L:145:LYS:HB3	1:L:197:THR:HB	1.91	0.52
2:H:55:TYR:OH	3:N:384:GLN:NE2	2.43	0.51
2:J:148:VAL:HG11	2:J:156:VAL:HG11	1.92	0.51
2:J:129:PRO:HD3	2:J:215:LYS:HE3	1.92	0.51
2:J:39:ILE:HD12	2:J:98:VAL:HG21	1.92	0.50
1:K:50:ASP:HB2	1:K:53:ASN:HD22	1.77	0.50
3:M:312:VAL:HG12	3:M:340:SER:HB3	1.92	0.50
1:K:137:ASN:HD21	2:J:170:HIS:HD2	1.59	0.50
1:L:137:ASN:HD21	2:H:170:HIS:CD2	2.31	0.48
3:N:442:ASN:H	3:N:469:ASN:ND2	2.12	0.48
3:N:369:ASP:OD1	3:N:390:ARG:NH1	2.46	0.47
3:N:440:SER:HA	3:N:467:ILE:O	2.15	0.47
1:L:42:LYS:NZ	4:L:304:SO4:O2	2.36	0.47
1:K:35:TRP:HB2	1:K:48:ILE:HB	1.96	0.46
3:N:489:GLU:OE1	3:N:501:SER:OG	2.31	0.46
2:J:8:GLY:HA3	2:J:20:LEU:HD23	1.97	0.45
2:J:40:ARG:HB3	2:J:50:ILE:HD11	1.99	0.45
1:K:47:LEU:HA	1:K:58:VAL:HG21	1.99	0.45
1:L:35:TRP:CE2	1:L:73:PHE:HB2	2.51	0.45
3:N:470:ARG:NH1	3:N:480:GLN:OE1	2.48	0.45
1:K:35:TRP:CE2	1:K:73:PHE:HB2	2.52	0.45
1:L:184:ALA:O	1:L:188:LYS:HG2	2.17	0.44
3:N:329:ALA:HA	3:N:363:LEU:HD13	1.99	0.44
2:J:35:TYR:HB2	2:J:100:ASP:HB3	1.99	0.44
3:M:345:LEU:HD11	3:M:381:LEU:HD13	1.99	0.43
3:M:476:LYS:HE3	3:M:476:LYS:HB2	1.87	0.43
2:J:29:VAL:HA	2:J:36:TRP:CZ2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:29:VAL:HA	2:H:36:TRP:CZ2	2.53	0.43
3:N:483:HIS:ND1	3:N:496:PRO:HG3	2.34	0.43
3:M:440:SER:HA	3:M:467:ILE:O	2.18	0.43
2:J:104:GLY:HA2	3:M:468:ARG:HH22	1.84	0.42
1:L:149:LYS:NZ	1:L:195:GLU:OE1	2.49	0.42
3:N:312:VAL:HG22	3:N:340:SER:HB3	2.00	0.42
1:L:47:LEU:HA	1:L:58:VAL:HG21	2.01	0.42
2:H:203:ASN:HB3	2:H:212:LYS:NZ	2.34	0.42
3:M:316:ILE:HD11	3:M:327:ILE:HG12	2.01	0.42
1:K:2:ILE:HD12	1:K:90:HIS:CE1	2.55	0.42
1:K:183:LYS:O	1:K:187:GLU:HG2	2.20	0.41
1:K:34:ASN:ND2	2:J:104:GLY:O	2.34	0.41
2:J:92:THR:HG23	2:J:116:THR:HA	2.03	0.41
2:J:17:THR:HA	2:J:85:SER:HA	2.03	0.41
1:L:183:LYS:O	1:L:187:GLU:HG2	2.21	0.41
3:M:403:ARG:O	3:M:433:SER:HB2	2.21	0.41
1:K:140:TYR:CG	1:K:141:PRO:HA	2.56	0.41
3:N:408:GLN:HG2	3:N:409:HIS:CD2	2.56	0.41
2:H:114:MET:HB2	7:H:304:1PE:H231	2.03	0.40
2:J:98:VAL:HG11	2:J:106:PHE:HB3	2.03	0.40
3:N:427:ARG:HA	3:N:492:TRP:CD1	2.57	0.40
2:J:165:LEU:HD21	2:J:188:VAL:HG11	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	211/214 (99%)	206 (98%)	5 (2%)	0	100	100
1	L	210/214 (98%)	205 (98%)	5 (2%)	0	100	100
2	H	201/221 (91%)	196 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	J	201/221 (91%)	196 (98%)	5 (2%)	0	100	100
3	M	192/201 (96%)	183 (95%)	9 (5%)	0	100	100
3	N	190/201 (94%)	183 (96%)	7 (4%)	0	100	100
All	All	1205/1272 (95%)	1169 (97%)	36 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	K	187/188 (100%)	187 (100%)	0	100	100
1	L	186/188 (99%)	186 (100%)	0	100	100
2	H	180/193 (93%)	180 (100%)	0	100	100
2	J	180/193 (93%)	178 (99%)	2 (1%)	65	84
3	M	169/176 (96%)	168 (99%)	1 (1%)	78	91
3	N	167/176 (95%)	167 (100%)	0	100	100
All	All	1069/1114 (96%)	1066 (100%)	3 (0%)	86	94

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	J	66	LYS
2	J	188	VAL
3	M	344	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	K	3	GLN
1	K	53	ASN

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Mol	Chain	Res	Type
1	K	79	GLN
1	K	137	ASN
1	K	138	ASN
2	J	1	GLN
2	J	58	ASN
1	L	3	GLN
1	L	53	ASN
2	H	5	GLN
2	H	60	ASN
2	H	170	HIS
3	M	346	HIS
3	M	384	GLN
3	M	398	ASN
3	M	409	HIS
3	M	444	ASN
3	M	480	GLN
3	N	384	GLN
3	N	449	ASN
3	N	469	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

22 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	$\# Z > 2$
6	EDO	H	306	-	3,3,3	0.43	0	2,2,2	0.40	0
4	SO4	L	305	-	4,4,4	0.23	0	6,6,6	0.06	0
4	SO4	L	302	-	4,4,4	0.24	0	6,6,6	0.07	0
6	EDO	J	302	-	3,3,3	0.41	0	2,2,2	0.39	0
6	EDO	K	306	-	3,3,3	0.43	0	2,2,2	0.36	0
7	1PE	H	304	-	15,15,15	0.55	0	14,14,14	0.23	0
4	SO4	H	303	-	4,4,4	0.24	0	6,6,6	0.07	0
4	SO4	L	301	-	4,4,4	0.24	0	6,6,6	0.08	0
5	GOL	K	304	-	5,5,5	0.38	0	5,5,5	0.28	0
5	GOL	K	305	-	5,5,5	0.38	0	5,5,5	0.33	0
7	1PE	L	306	-	15,15,15	0.54	0	14,14,14	0.23	0
4	SO4	L	304	-	4,4,4	0.24	0	6,6,6	0.08	0
4	SO4	H	302	-	4,4,4	0.24	0	6,6,6	0.08	0
5	GOL	H	305	-	5,5,5	0.37	0	5,5,5	0.35	0
4	SO4	N	601	-	4,4,4	0.23	0	6,6,6	0.07	0
4	SO4	H	301	-	4,4,4	0.24	0	6,6,6	0.08	0
4	SO4	K	302	-	4,4,4	0.24	0	6,6,6	0.07	0
4	SO4	K	301	-	4,4,4	0.24	0	6,6,6	0.07	0
4	SO4	L	303	-	4,4,4	0.24	0	6,6,6	0.08	0
4	SO4	K	303	-	4,4,4	0.23	0	6,6,6	0.08	0
5	GOL	L	307	-	5,5,5	0.36	0	5,5,5	0.32	0
7	1PE	J	301	-	15,15,15	0.54	0	14,14,14	0.21	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
7	1PE	L	306	-	-	10/13/13/13	-
6	EDO	K	306	-	-	0/1/1/1	-
6	EDO	H	306	-	-	0/1/1/1	-
7	1PE	H	304	-	-	6/13/13/13	-
5	GOL	H	305	-	-	2/4/4/4	-
6	EDO	J	302	-	-	0/1/1/1	-
5	GOL	L	307	-	-	2/4/4/4	-
5	GOL	K	304	-	-	2/4/4/4	-
5	GOL	K	305	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	1PE	J	301	-	-	7/13/13/13	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	K	305	GOL	O1-C1-C2-C3
5	L	307	GOL	O1-C1-C2-C3
5	H	305	GOL	O1-C1-C2-C3
7	H	304	1PE	OH6-C15-C25-OH5
7	H	304	1PE	OH4-C13-C23-OH3
7	L	306	1PE	OH4-C13-C23-OH3
7	J	301	1PE	OH6-C15-C25-OH5
5	K	304	GOL	O1-C1-C2-C3
7	L	306	1PE	OH6-C15-C25-OH5
5	K	305	GOL	O1-C1-C2-O2
7	H	304	1PE	OH2-C12-C22-OH3
5	L	307	GOL	O1-C1-C2-O2
5	H	305	GOL	O1-C1-C2-O2
7	L	306	1PE	OH7-C16-C26-OH6
7	J	301	1PE	OH4-C13-C23-OH3
5	K	304	GOL	O1-C1-C2-O2
7	H	304	1PE	C12-C22-OH3-C23
7	J	301	1PE	C23-C13-OH4-C24
7	L	306	1PE	C12-C22-OH3-C23
7	L	306	1PE	C13-C23-OH3-C22
7	L	306	1PE	C16-C26-OH6-C15
7	L	306	1PE	C24-C14-OH5-C25
7	H	304	1PE	C15-C25-OH5-C14
7	L	306	1PE	C23-C13-OH4-C24
7	L	306	1PE	C14-C24-OH4-C13
7	J	301	1PE	OH5-C14-C24-OH4
7	J	301	1PE	C24-C14-OH5-C25
7	J	301	1PE	C15-C25-OH5-C14
7	J	301	1PE	C12-C22-OH3-C23
7	H	304	1PE	C23-C13-OH4-C24
7	L	306	1PE	OH5-C14-C24-OH4

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	H	304	1PE	1	0
5	K	304	GOL	1	0
4	L	304	SO4	1	0
4	K	303	SO4	1	0
7	J	301	1PE	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	K	213/214 (99%)	0.03	6 (2%) 55 50	21, 37, 59, 105	0
1	L	212/214 (99%)	-0.01	3 (1%) 73 70	19, 36, 56, 74	0
2	H	207/221 (93%)	0.26	10 (4%) 35 31	22, 39, 72, 108	0
2	J	207/221 (93%)	0.51	17 (8%) 17 15	23, 45, 85, 111	0
3	M	194/201 (96%)	1.99	78 (40%) 0 0	50, 86, 128, 178	0
3	N	192/201 (95%)	1.66	63 (32%) 1 1	51, 81, 112, 129	0
All	All	1225/1272 (96%)	0.71	177 (14%) 6 5	19, 46, 106, 178	0

All (177) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	M	472	GLU	5.9
3	N	500	VAL	5.8
3	M	329	ALA	5.7
3	M	310	LYS	5.6
3	M	319	GLY	5.6
3	N	485	LEU	5.4
3	M	318	ILE	5.3
2	J	134	SER	4.9
3	N	501	SER	4.7
1	K	212	GLY	4.6
3	M	486	CYS	4.6
3	M	501	SER	4.5
3	M	500	VAL	4.5
3	M	485	LEU	4.4
2	J	44	GLY	4.4
3	M	320	GLU	4.3
3	M	359	HIS	4.3
3	M	315	GLY	4.3
3	N	472	GLU	4.2

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Mol	Chain	Res	Type	RSRZ
3	M	490	GLY	4.2
3	N	489	GLU	4.1
3	M	311	LYS	4.0
3	M	337	ASN	3.9
3	M	366	GLN	3.9
3	M	389	ASN	3.8
3	M	353	ARG	3.7
3	M	335	PHE	3.7
3	N	320	GLU	3.7
3	M	343	GLY	3.7
2	H	141	THR	3.7
2	J	76	SER	3.7
2	J	191	PRO	3.7
3	M	1502	HIS	3.6
3	M	357	PHE	3.6
3	M	362	PRO	3.6
3	M	322	LYS	3.5
3	N	499	CYS	3.5
3	M	324	SER	3.5
3	M	345	LEU	3.5
3	M	365	PRO	3.5
3	M	361	PRO	3.5
2	J	140	SER	3.5
3	M	312	VAL	3.4
3	M	368	LEU	3.3
3	N	490	GLY	3.3
3	N	366	GLN	3.2
3	N	318	ILE	3.2
3	M	358	THR	3.2
3	M	370	ILE	3.2
3	N	343	GLY	3.1
3	M	388	GLU	3.1
2	H	23	THR	3.1
2	J	30	SER	3.1
3	N	460	SER	3.1
3	M	373	THR	3.1
3	N	459	THR	3.0
3	M	351	ALA	3.0
3	N	390	ARG	3.0
3	M	495	GLU	3.0
3	N	430	LYS	3.0
3	N	312	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
3	N	358	THR	3.0
2	J	23	THR	2.9
3	N	488	PRO	2.9
3	M	321	PHE	2.9
3	N	449	ASN	2.9
3	M	430	LYS	2.9
3	N	368	LEU	2.9
1	L	212	GLY	2.9
3	M	333	LYS	2.9
3	N	453	TRP	2.9
3	N	388	GLU	2.9
3	M	313	CYS	2.8
3	M	499	CYS	2.8
3	M	352	PHE	2.8
3	M	1503	HIS	2.8
1	K	1	ASP	2.8
2	H	192	SER	2.8
3	N	370	ILE	2.7
3	M	487	SER	2.7
2	J	29	VAL	2.7
3	N	363	LEU	2.7
3	N	310	LYS	2.7
3	M	330	THR	2.7
3	N	448	ALA	2.7
3	N	484	ALA	2.7
2	J	31	SER	2.7
3	M	386	TRP	2.7
3	M	497	ARG	2.7
3	N	464	THR	2.7
3	M	425	GLY	2.7
3	M	336	LYS	2.7
3	M	477	ALA	2.7
3	M	328	ASP	2.6
3	N	461	GLY	2.6
3	M	460	SER	2.6
3	M	317	GLY	2.6
3	N	446	CYS	2.6
3	N	337	ASN	2.6
3	N	394	HIS	2.6
3	M	323	ASP	2.6
2	H	1	GLN	2.6
3	N	327	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
3	N	357	PHE	2.6
3	M	327	ILE	2.5
3	M	390	ARG	2.5
2	H	191	PRO	2.5
3	N	458	GLY	2.5
3	N	350	VAL	2.5
3	N	351	ALA	2.5
3	M	381	LEU	2.5
3	M	350	VAL	2.5
3	M	427	ARG	2.5
3	N	389	ASN	2.5
3	N	329	ALA	2.5
3	N	315	GLY	2.4
3	M	338	CYS	2.4
3	N	333	LYS	2.4
3	M	363	LEU	2.4
3	N	324	SER	2.4
3	M	341	ILE	2.4
3	M	371	LEU	2.4
3	N	452	ASN	2.4
1	L	169	LYS	2.4
3	M	428	SER	2.4
3	N	495	GLU	2.4
2	J	75	THR	2.3
3	N	491	CYS	2.3
3	M	496	PRO	2.3
3	M	394	HIS	2.3
3	N	438	ILE	2.3
3	N	481	VAL	2.3
3	N	319	GLY	2.3
3	N	487	SER	2.3
3	N	334	HIS	2.3
3	N	325	LEU	2.3
2	J	103	THR	2.3
2	H	124	GLY	2.3
2	H	134	SER	2.3
2	J	77	LYS	2.3
1	K	187	GLU	2.3
3	M	334	HIS	2.2
3	N	371	LEU	2.2
2	J	218	GLU	2.2
3	N	397	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
3	M	349	PRO	2.2
1	K	152	ASN	2.2
3	N	401	ILE	2.2
3	N	322	LYS	2.2
3	N	359	HIS	2.2
3	N	313	CYS	2.2
3	N	321	PHE	2.2
3	M	398	ASN	2.1
3	N	314	ASN	2.1
2	H	74	ASP	2.1
1	L	152	ASN	2.1
3	M	424	LEU	2.1
3	N	317	GLY	2.1
3	M	449	ASN	2.1
1	K	83	ILE	2.1
3	N	338	CYS	2.1
2	J	198	GLN	2.1
3	N	410	GLY	2.1
3	M	378	THR	2.1
2	H	66	LYS	2.1
3	M	364	ASP	2.1
3	M	434	ASP	2.1
2	J	104	GLY	2.0
2	H	103	THR	2.0
3	M	339	THR	2.0
3	N	377	ILE	2.0
3	M	483	HIS	2.0
2	J	1	GLN	2.0
1	K	107	LYS	2.0
3	M	375	LYS	2.0
3	M	360	THR	2.0
2	J	74	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SO4	N	601	5/5	0.64	0.16	97,97,99,100	0
4	SO4	L	303	5/5	0.69	0.12	109,111,111,113	0
4	SO4	K	302	5/5	0.71	0.19	94,97,98,103	0
4	SO4	L	301	5/5	0.72	0.29	89,91,97,97	0
4	SO4	H	303	5/5	0.77	0.18	87,90,94,96	0
4	SO4	L	302	5/5	0.77	0.31	92,93,96,96	0
7	1PE	L	306	16/16	0.81	0.19	50,59,67,68	0
4	SO4	H	301	5/5	0.82	0.24	89,93,96,97	0
7	1PE	J	301	16/16	0.83	0.16	44,54,68,69	0
5	GOL	K	305	6/6	0.83	0.19	55,57,59,62	0
4	SO4	L	305	5/5	0.84	0.15	68,71,76,77	0
5	GOL	L	307	6/6	0.85	0.16	44,56,57,57	0
5	GOL	K	304	6/6	0.86	0.14	48,53,56,57	0
5	GOL	H	305	6/6	0.86	0.16	51,54,57,60	0
4	SO4	K	303	5/5	0.87	0.11	74,79,80,81	0
6	EDO	K	306	4/4	0.87	0.14	41,43,47,47	0
4	SO4	L	304	5/5	0.89	0.11	69,72,77,79	0
6	EDO	J	302	4/4	0.89	0.15	47,49,52,56	0
4	SO4	H	302	5/5	0.90	0.19	92,94,96,98	0
7	1PE	H	304	16/16	0.90	0.12	34,49,56,60	0
4	SO4	K	301	5/5	0.93	0.11	66,68,73,74	0
6	EDO	H	306	4/4	0.95	0.12	46,47,48,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.