



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 24, 2023 – 12:18 AM EDT

PDB ID : 5SX5
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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

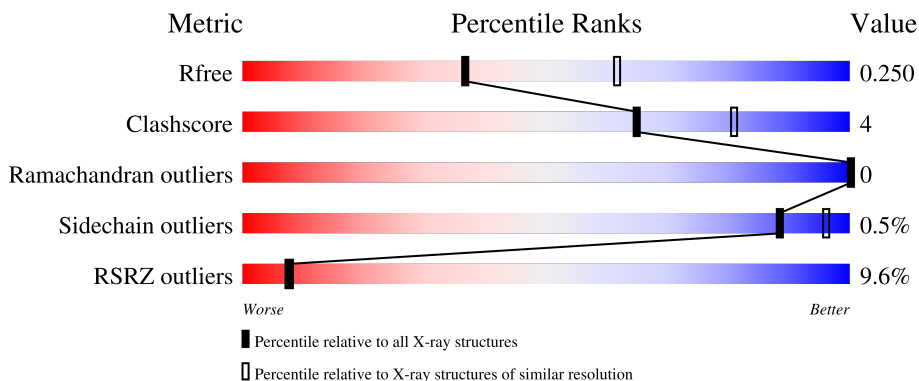
1 Overall quality at a glance

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.



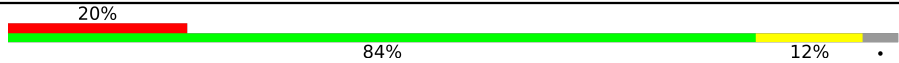
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	 2% 89% 10%
1	L	214	 % 89% 10% .
2	H	221	 2% 88% 5% 6%
2	J	221	 6% 79% 14% 6%
3	M	201	 26% 87% 9% .

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Mol	Chain	Length	Quality of chain
3	N	201	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into three segments: a red segment on the left labeled '20%', a large green segment in the middle labeled '84%', and a yellow segment on the right labeled '12%'. A small grey dot is visible at the far right end of the bar.</p>

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
			Total	C	N	O	S			
1	K	213	Total 1637	C 1025	N 273	O 334	S 5	0	0	0
1	L	212	Total 1628	C 1020	N 272	O 331	S 5	0	0	0

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

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

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

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

There are 26 discrepancies between the modelled and reference sequences:

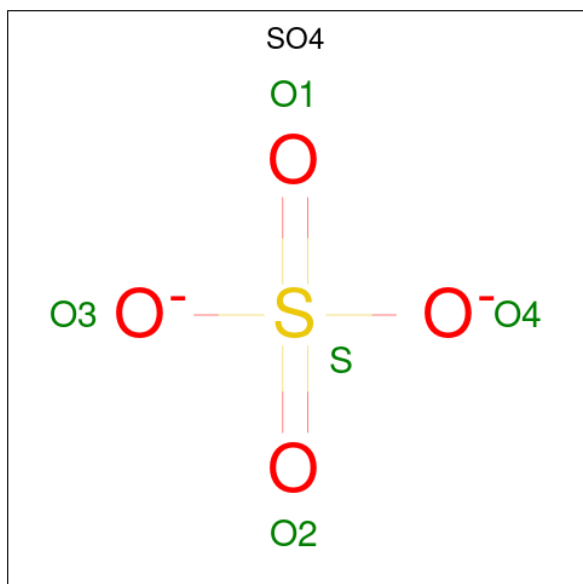
Chain	Residue	Modelled	Actual	Comment	Reference
M	307	LEU	-	expression tag	UNP P00533
M	308	GLU	-	expression tag	UNP P00533
M	309	GLU	-	expression tag	UNP P00533
M	310	LYS	-	expression tag	UNP P00533
M	328	ASP	ASN	conflict	UNP P00533
M	420	ASP	ASN	conflict	UNP P00533
M	468	ARG	SER	engineered mutation	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 (three-letter code: SO4) (formula: O₄S).



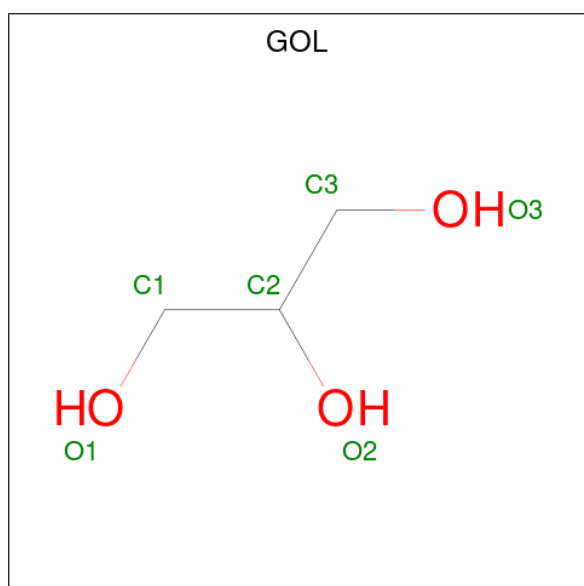
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	K	1	Total O S 5 4 1	0	0
4	K	1	Total O S 5 4 1	0	0

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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	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 (three-letter code: GOL) (formula: C₃H₈O₃).



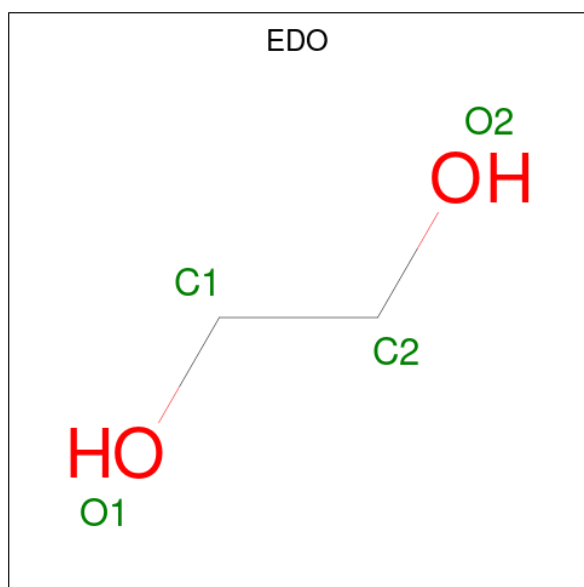
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	K	1	Total	C	O	0	0
			6	3	3		

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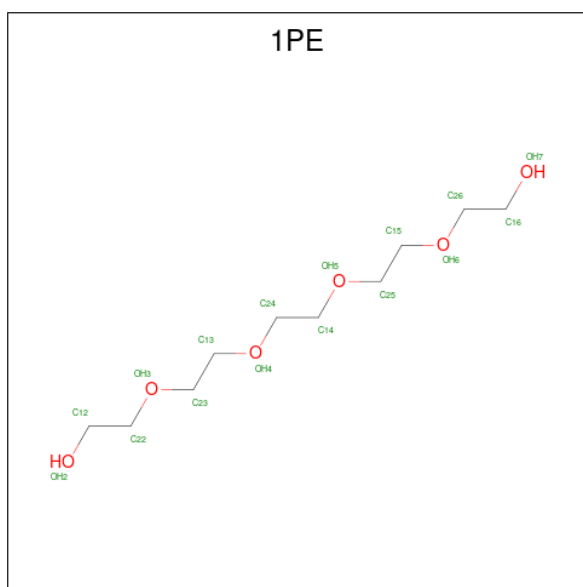
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	K	1	Total	C	O	0	0
			6	3	3		
5	L	1	Total	C	O	0	0
			6	3	3		
5	H	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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 (three-letter code: 1PE) (formula: C₁₀H₂₂O₆).



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		

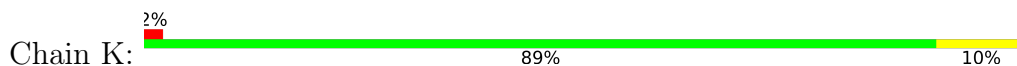
- Molecule 8 is water.

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		

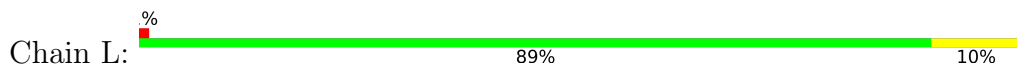
3 Residue-property plots [i](#)

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.

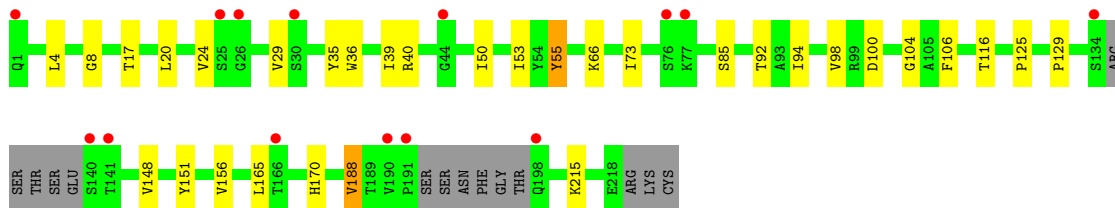
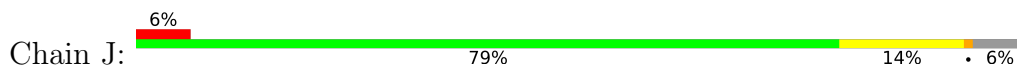
- Molecule 1: Panitumumab Fab Light Chain



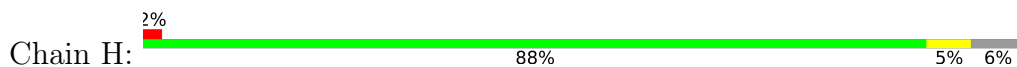
- Molecule 1: Panitumumab Fab Light Chain



- Molecule 2: Panitumumab Fab Heavy Chain

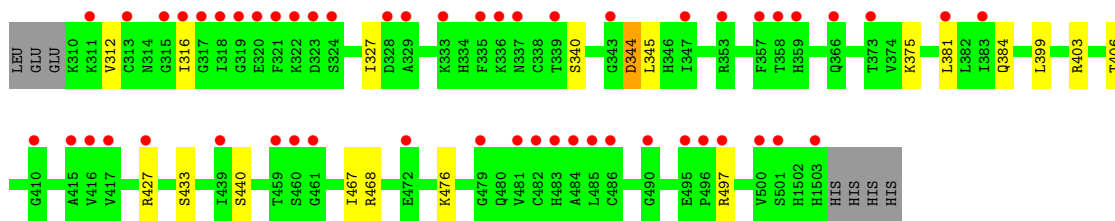


- Molecule 2: Panitumumab Fab Heavy Chain

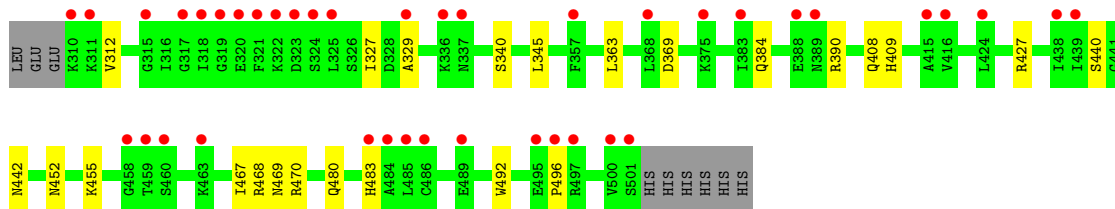
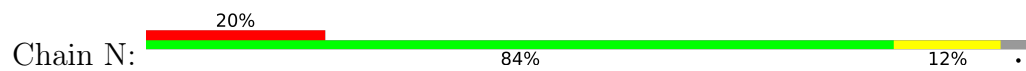


- Molecule 3: Epidermal growth factor receptor





- 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)	Xtrriage
Refinement program	PHENIX dev_2356	Depositor
R, R_{free}	0.226 , 0.250 0.226 , 0.250	Depositor DCC
R_{free} test set	2687 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	35.2	Xtrriage
Anisotropy	0.077	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 42.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 1PE, SO4, EDO, GOL

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	0.25	0/1673	0.45	0/2272
1	L	0.25	0/1664	0.46	0/2260
2	H	0.25	0/1593	0.47	0/2177
2	J	0.25	0/1593	0.48	0/2177
3	M	0.24	0/1532	0.45	0/2070
3	N	0.24	0/1510	0.43	0/2040
All	All	0.25	0/9565	0.46	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 [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	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	17	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	77	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 (77) 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
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
1:K:45:LYS:NZ	8:K:404:HOH:O	2.42	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
2:H:29:VAL:HA	2:H:36:TRP:CZ2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2	J	201/221 (91%)	196 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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 [\(i\)](#)

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%)	179 (99%)	1 (1%)	86	95
2	J	180/193 (93%)	177 (98%)	3 (2%)	60	82
3	M	169/176 (96%)	168 (99%)	1 (1%)	86	95
3	N	167/176 (95%)	167 (100%)	0	100	100
All	All	1069/1114 (96%)	1064 (100%)	5 (0%)	88	96

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	J	55	TYR
2	J	66	LYS
2	J	188	VAL
2	H	55	TYR
3	M	344	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) 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	137	ASN
1	K	138	ASN
2	J	1	GLN
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	N	384	GLN
3	N	398	ASN
3	N	469	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
7	1PE	H	304	-	15,15,15	0.53	0	14,14,14	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	K	303	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	N	601	-	4,4,4	0.14	0	6,6,6	0.05	0
7	1PE	L	306	-	15,15,15	0.53	0	14,14,14	0.23	0
4	SO4	K	301	-	4,4,4	0.14	0	6,6,6	0.04	0
4	SO4	H	302	-	4,4,4	0.14	0	6,6,6	0.05	0
6	EDO	H	306	-	3,3,3	0.46	0	2,2,2	0.36	0
4	SO4	K	302	-	4,4,4	0.14	0	6,6,6	0.05	0
5	GOL	L	307	-	5,5,5	0.36	0	5,5,5	0.28	0
4	SO4	L	303	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	L	304	-	4,4,4	0.14	0	6,6,6	0.04	0
4	SO4	H	303	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	L	301	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	L	305	-	4,4,4	0.14	0	6,6,6	0.05	0
5	GOL	K	304	-	5,5,5	0.37	0	5,5,5	0.25	0
5	GOL	K	305	-	5,5,5	0.38	0	5,5,5	0.29	0
4	SO4	L	302	-	4,4,4	0.14	0	6,6,6	0.05	0
7	1PE	J	301	-	15,15,15	0.53	0	14,14,14	0.22	0
4	SO4	H	301	-	4,4,4	0.14	0	6,6,6	0.05	0
6	EDO	K	306	-	3,3,3	0.46	0	2,2,2	0.32	0
6	EDO	J	302	-	3,3,3	0.45	0	2,2,2	0.35	0
5	GOL	H	305	-	5,5,5	0.36	0	5,5,5	0.31	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	1PE	H	304	-	-	7/13/13/13	-
6	EDO	K	306	-	-	0/1/1/1	-
5	GOL	K	304	-	-	2/4/4/4	-
5	GOL	L	307	-	-	2/4/4/4	-
5	GOL	K	305	-	-	2/4/4/4	-
6	EDO	J	302	-	-	0/1/1/1	-
7	1PE	L	306	-	-	10/13/13/13	-
7	1PE	J	301	-	-	7/13/13/13	-
6	EDO	H	306	-	-	0/1/1/1	-
5	GOL	H	305	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	K	304	GOL	O1-C1-C2-C3
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
7	L	306	1PE	OH6-C15-C25-OH5
7	H	304	1PE	OH2-C12-C22-OH3
5	K	305	GOL	O1-C1-C2-O2
7	J	301	1PE	OH4-C13-C23-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
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	C16-C26-OH6-C15
7	L	306	1PE	C13-C23-OH3-C22
7	L	306	1PE	C24-C14-OH5-C25
7	H	304	1PE	C15-C25-OH5-C14
7	L	306	1PE	C14-C24-OH4-C13
7	L	306	1PE	C23-C13-OH4-C24
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	H	304	1PE	C23-C13-OH4-C24
7	L	306	1PE	OH5-C14-C24-OH4
7	J	301	1PE	C12-C22-OH3-C23
7	H	304	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
4	K	303	SO4	1	0
4	L	304	SO4	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	K	304	GOL	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%)	-0.09	4 (1%) 66 69	21, 37, 59, 105	0
1	L	212/214 (99%)	-0.10	2 (0%) 84 86	19, 36, 56, 74	0
2	H	207/221 (93%)	0.02	5 (2%) 59 62	22, 39, 72, 108	0
2	J	207/221 (93%)	0.20	14 (6%) 17 17	23, 45, 85, 111	0
3	M	194/201 (96%)	1.54	53 (27%) 0 0	50, 86, 128, 178	0
3	N	192/201 (95%)	1.20	40 (20%) 1 0	51, 81, 112, 129	0
All	All	1225/1272 (96%)	0.44	118 (9%) 8 7	19, 46, 106, 178	0

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	N	485	LEU	10.4
3	M	318	ILE	8.6
3	M	319	GLY	8.5
3	M	329	ALA	5.7
3	M	486	CYS	5.7
3	M	485	LEU	5.5
3	M	320	GLU	5.1
3	M	337	ASN	4.9
3	N	484	ALA	4.8
3	M	315	GLY	4.7
2	H	1	GLN	4.4
3	N	319	GLY	4.4
3	N	318	ILE	4.4
3	M	496	PRO	4.3
3	M	460	SER	4.3
3	M	366	GLN	4.2
3	M	357	PHE	4.2
3	M	472	GLU	4.1
3	M	324	SER	4.1

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Mol	Chain	Res	Type	RSRZ
3	N	323	ASP	4.1
3	M	417	VAL	4.1
3	M	484	ALA	4.0
3	N	415	ALA	3.9
3	N	315	GLY	3.8
3	M	495	GLU	3.8
3	M	323	ASP	3.8
3	N	495	GLU	3.8
3	N	389	ASN	3.8
2	J	134	SER	3.8
2	J	140	SER	3.7
3	N	310	LYS	3.7
3	N	311	LYS	3.7
3	N	325	LEU	3.7
3	M	383	ILE	3.5
3	M	500	VAL	3.5
3	M	339	THR	3.4
3	N	324	SER	3.4
3	M	322	LYS	3.4
3	N	458	GLY	3.4
1	K	212	GLY	3.3
3	M	410	GLY	3.3
3	M	483	HIS	3.2
2	J	190	VAL	3.2
3	N	460	SER	3.2
2	H	192	SER	3.2
3	N	337	ASN	3.1
3	M	353	ARG	3.1
3	N	463	LYS	3.1
3	M	461	GLY	3.0
3	N	497	ARG	3.0
3	M	416	VAL	3.0
3	M	333	LYS	2.9
3	N	317	GLY	2.9
3	M	311	LYS	2.9
3	M	482	CYS	2.9
3	M	490	GLY	2.9
2	J	198	GLN	2.9
3	M	373	THR	2.9
3	M	459	THR	2.9
3	M	497	ARG	2.8
3	M	335	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
2	J	77	LYS	2.8
3	N	320	GLU	2.7
3	N	500	VAL	2.7
3	M	313	CYS	2.7
2	J	1	GLN	2.7
3	N	416	VAL	2.7
3	N	501	SER	2.7
3	M	1503	HIS	2.7
3	N	321	PHE	2.6
3	N	439	ILE	2.6
1	K	188	LYS	2.6
2	H	77	LYS	2.6
2	J	191	PRO	2.6
2	J	30	SER	2.6
3	M	321	PHE	2.6
3	N	483	HIS	2.6
3	N	336	LYS	2.5
3	M	439	ILE	2.5
2	J	26	GLY	2.5
3	N	357	PHE	2.5
3	N	438	ILE	2.5
3	M	501	SER	2.5
3	M	381	LEU	2.5
2	J	166	THR	2.5
3	M	316	ILE	2.4
3	N	322	LYS	2.4
2	J	76	SER	2.4
3	M	481	VAL	2.4
1	K	187	GLU	2.4
3	M	359	HIS	2.4
2	J	141	THR	2.4
3	N	424	LEU	2.3
3	N	375	LYS	2.3
3	N	486	CYS	2.3
3	M	328	ASP	2.3
3	M	358	THR	2.3
1	L	190	LYS	2.2
3	M	317	GLY	2.2
1	L	56	THR	2.2
2	H	191	PRO	2.2
2	J	44	GLY	2.2
3	M	415	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
3	N	459	THR	2.2
3	N	329	ALA	2.2
3	M	479	GLY	2.1
3	N	368	LEU	2.1
3	M	347	ILE	2.1
3	M	427	ARG	2.1
2	H	26	GLY	2.1
3	N	383	ILE	2.1
3	N	388	GLU	2.1
3	M	343	GLY	2.1
3	M	336	LYS	2.1
1	K	126	LYS	2.1
2	J	25	SER	2.0
3	N	496	PRO	2.0
3	N	489	GLU	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 monosaccharides 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	L	303	5/5	0.81	0.47	109,111,111,113	0
4	SO4	H	301	5/5	0.83	0.45	89,93,96,97	0
5	GOL	K	305	6/6	0.84	0.25	55,57,59,62	0
7	1PE	L	306	16/16	0.84	0.24	50,59,67,68	0
4	SO4	K	302	5/5	0.85	0.41	94,97,98,103	0
5	GOL	H	305	6/6	0.86	0.26	51,54,57,60	0
4	SO4	N	601	5/5	0.86	0.51	97,97,99,100	0
5	GOL	L	307	6/6	0.87	0.18	44,56,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	SO4	L	301	5/5	0.87	0.37	89,91,97,97	0
4	SO4	L	302	5/5	0.87	0.47	92,93,96,96	0
6	EDO	K	306	4/4	0.88	0.20	41,43,47,47	0
7	1PE	J	301	16/16	0.89	0.18	44,54,68,69	0
4	SO4	H	303	5/5	0.90	0.30	87,90,94,96	0
4	SO4	H	302	5/5	0.90	0.25	92,94,96,98	0
7	1PE	H	304	16/16	0.92	0.17	34,49,56,60	0
5	GOL	K	304	6/6	0.93	0.13	48,53,56,57	0
4	SO4	L	305	5/5	0.94	0.15	68,71,76,77	0
4	SO4	K	303	5/5	0.94	0.18	74,79,80,81	0
6	EDO	H	306	4/4	0.94	0.17	46,47,48,51	0
4	SO4	L	304	5/5	0.95	0.12	69,72,77,79	0
6	EDO	J	302	4/4	0.95	0.11	47,49,52,56	0
4	SO4	K	301	5/5	0.97	0.13	66,68,73,74	0

6.5 Other polymers [i](#)

There are no such residues in this entry.