Full wwPDB X-ray Structure Validation Report (i)

Sep 28, 2016 – 04:50 PM 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

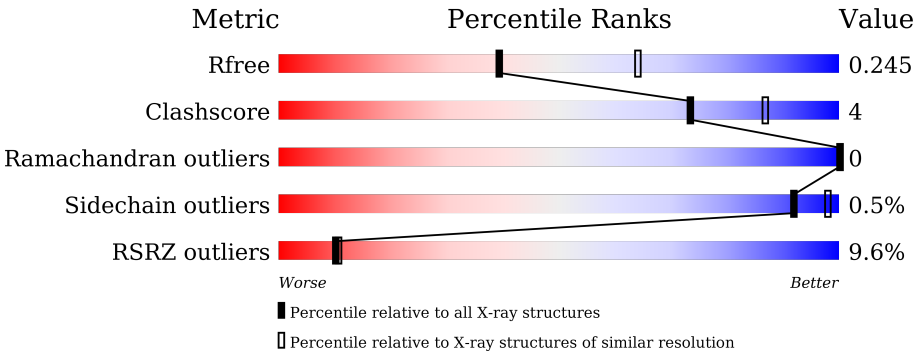
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

1 Overall quality at a glance (i)

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}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	2% 89% 10%
2	H	221	2% 88% 5% 6%
2	J	221	6% 79% 14% 6%
3	M	201	26% 87% 9%
3	N	201	20% 84% 12%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	N	601	-	-	-	X
5	GOL	H	305	-	-	-	X
5	GOL	K	305	-	-	-	X
7	1PE	L	306	-	-	-	X

2 Entry composition

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:

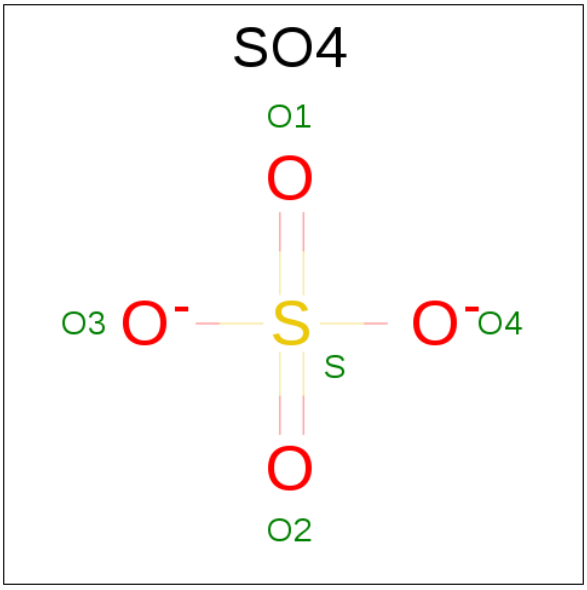
Chain	Residue	Modelled	Actual	Comment	Reference
M	307	LEU	-	expression tag	UNP P00533
M	308	GLU	-	expression tag	UNP P00533
M	309	GLU	-	expression tag	UNP P00533
M	310	LYS	-	expression tag	UNP P00533
M	328	ASP	ASN	conflict	UNP P00533
M	420	ASP	ASN	conflict	UNP P00533
M	468	ARG	SER	engineered mutation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

Continued on next page...

Continued from previous page...

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: O_4S).



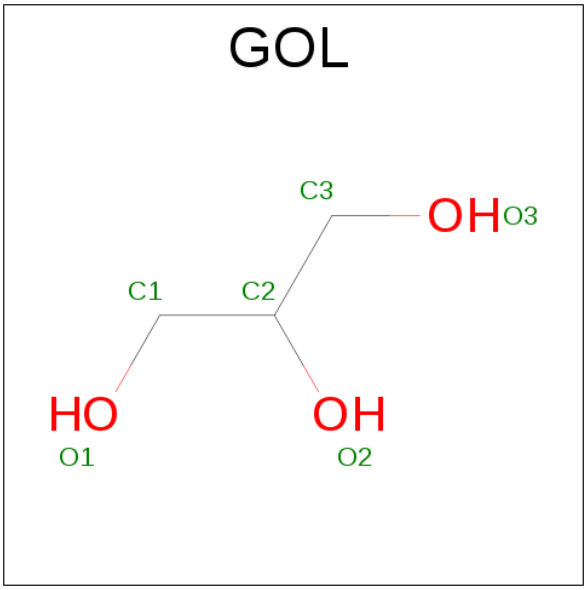
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	K	1	Total O S 5 4 1	0	0
4	K	1	Total O S 5 4 1	0	0

Continued on next page...

Continued from previous page...

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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



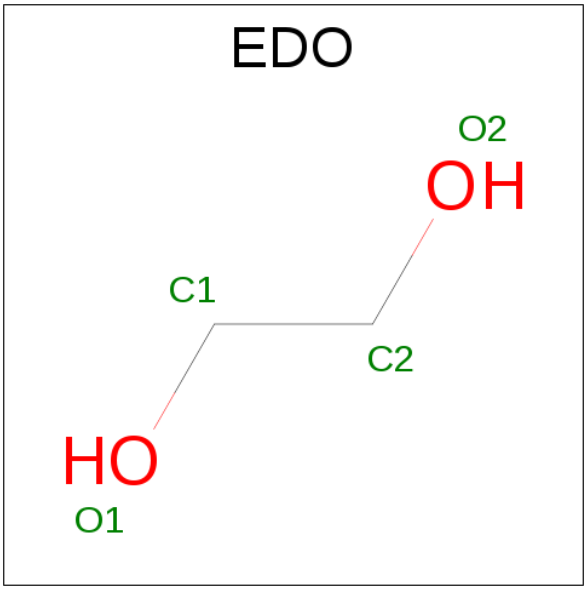
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	K	1	Total C O 6 3 3	0	0

Continued on next page...

Continued from previous page...

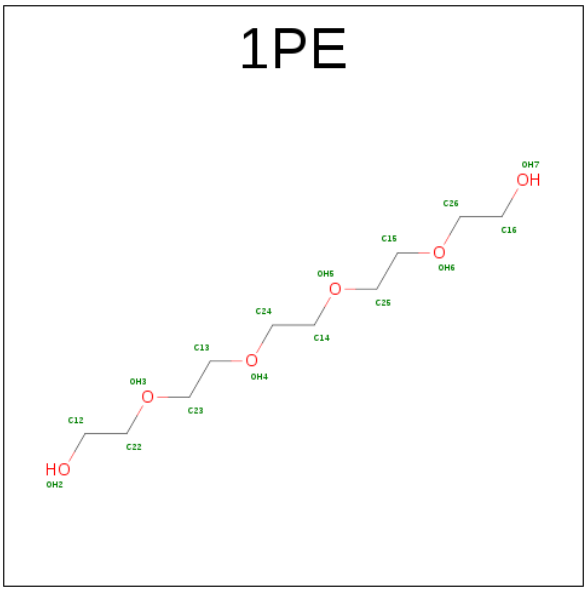
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	K	1	Total C O 6 3 3	0	0
5	L	1	Total C O 6 3 3	0	0
5	H	1	Total C O 6 3 3	0	0

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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



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

- Molecule 8 is water.

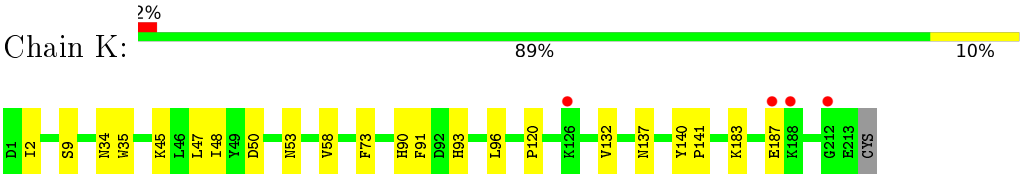
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	K	43	Total O 43 43	0	0
8	J	21	Total O 21 21	0	0
8	L	38	Total O 38 38	0	0
8	H	30	Total O 30 30	0	0
8	M	4	Total O 4 4	0	0
8	N	3	Total O 3 3	0	0

3 Residue-property plots (i)

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.

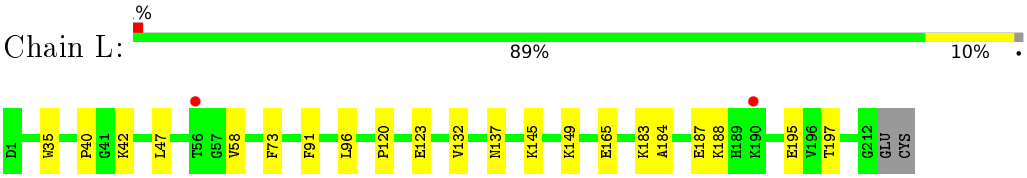
- Molecule 1: Panitumumab Fab Light Chain

Chain K:



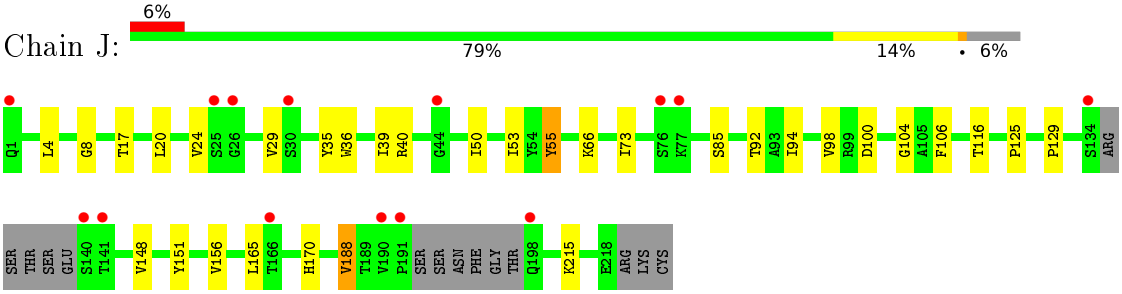
- Molecule 1: Panitumumab Fab Light Chain

Chain L:



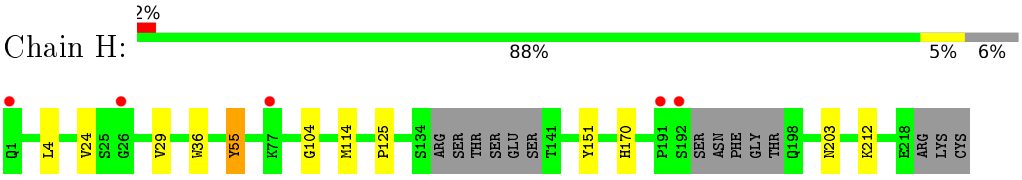
- Molecule 2: Panitumumab Fab Heavy Chain

Chain J:



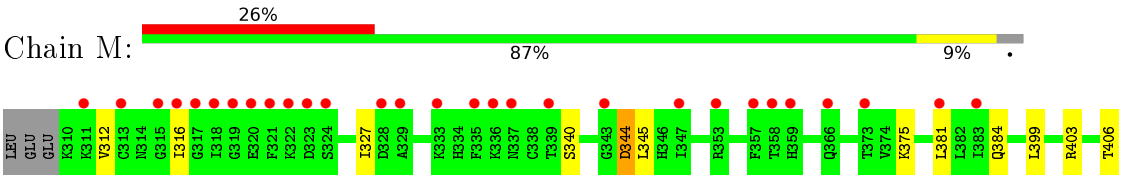
- Molecule 2: Panitumumab Fab Heavy Chain

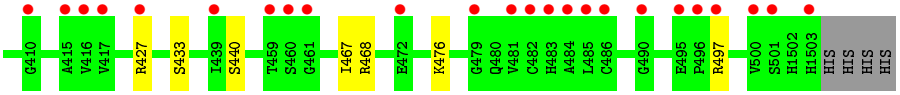
Chain H:



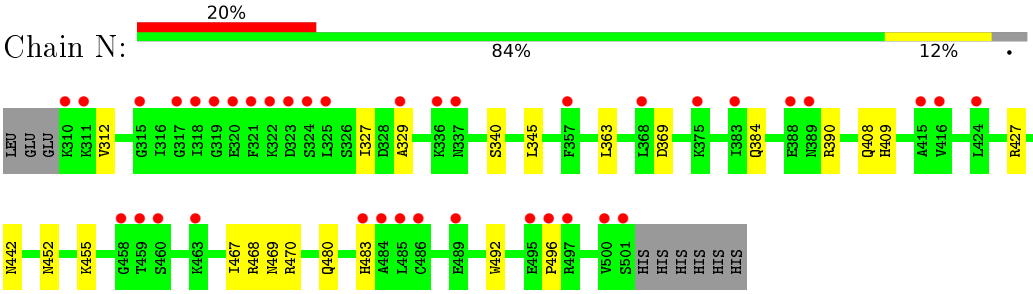
- Molecule 3: Epidermal growth factor receptor

Chain M:





- Molecule 3: Epidermal growth factor receptor



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	3.42 (at 2.51Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.226 , 0.250 0.216 , 0.245	Depositor DCC
R_{free} test set	2567 reflections (4.90%)	DCC
Wilson B-factor (Å^2)	36.1	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 42.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	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 19.56% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: GOL, 1PE, 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	0.25	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

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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:N	1:L:123:GLU:OE1	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:HB2	3:M:476:LYS:HE3	1.87	0.43
2:H:29:VAL:HA	2:H:36:TRP:CZ2	2.53	0.43
2:J:29:VAL:HA	2:J:36:TRP:CZ2	2.53	0.43

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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%)	90	97
2	J	180/193 (93%)	177 (98%)	3 (2%)	68	89
3	M	169/176 (96%)	168 (99%)	1 (1%)	90	97
3	N	167/176 (95%)	167 (100%)	0	100	100
All	All	1069/1114 (96%)	1064 (100%)	5 (0%)	92	98

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

Some 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

Continued on next page...

Continued from previous page...

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

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 carbohydrates 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	$\#\|Z\| > 2$
4	SO4	H	301	-	4,4,4	0.24	0	6,6,6	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	SO4	H	302	-	4,4,4	0.23	0	6,6,6	0.07	0
4	SO4	H	303	-	4,4,4	0.23	0	6,6,6	0.07	0
7	1PE	H	304	-	15,15,15	0.55	0	14,14,14	0.25	0
5	GOL	H	305	-	5,5,5	0.36	0	5,5,5	0.24	0
6	EDO	H	306	-	3,3,3	0.45	0	2,2,2	0.42	0
7	1PE	J	301	-	15,15,15	0.55	0	14,14,14	0.23	0
6	EDO	J	302	-	3,3,3	0.43	0	2,2,2	0.42	0
4	SO4	K	301	-	4,4,4	0.24	0	6,6,6	0.06	0
4	SO4	K	302	-	4,4,4	0.24	0	6,6,6	0.06	0
4	SO4	K	303	-	4,4,4	0.24	0	6,6,6	0.07	0
5	GOL	K	304	-	5,5,5	0.36	0	5,5,5	0.22	0
5	GOL	K	305	-	5,5,5	0.37	0	5,5,5	0.23	0
6	EDO	K	306	-	3,3,3	0.45	0	2,2,2	0.38	0
4	SO4	L	301	-	4,4,4	0.24	0	6,6,6	0.07	0
4	SO4	L	302	-	4,4,4	0.24	0	6,6,6	0.07	0
4	SO4	L	303	-	4,4,4	0.25	0	6,6,6	0.07	0
4	SO4	L	304	-	4,4,4	0.24	0	6,6,6	0.06	0
4	SO4	L	305	-	4,4,4	0.25	0	6,6,6	0.06	0
7	1PE	L	306	-	15,15,15	0.55	0	14,14,14	0.25	0
5	GOL	L	307	-	5,5,5	0.34	0	5,5,5	0.23	0
4	SO4	N	601	-	4,4,4	0.24	0	6,6,6	0.06	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
4	SO4	H	301	-	-	0/0/0/0	0/0/0/0
4	SO4	H	302	-	-	0/0/0/0	0/0/0/0
4	SO4	H	303	-	-	0/0/0/0	0/0/0/0
7	1PE	H	304	-	-	0/13/13/13	0/0/0/0
5	GOL	H	305	-	-	0/4/4/4	0/0/0/0
6	EDO	H	306	-	-	0/1/1/1	0/0/0/0
7	1PE	J	301	-	-	0/13/13/13	0/0/0/0
6	EDO	J	302	-	-	0/1/1/1	0/0/0/0
4	SO4	K	301	-	-	0/0/0/0	0/0/0/0
4	SO4	K	302	-	-	0/0/0/0	0/0/0/0
4	SO4	K	303	-	-	0/0/0/0	0/0/0/0
5	GOL	K	304	-	-	0/4/4/4	0/0/0/0
5	GOL	K	305	-	-	0/4/4/4	0/0/0/0
6	EDO	K	306	-	-	0/1/1/1	0/0/0/0
4	SO4	L	301	-	-	0/0/0/0	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SO4	L	302	-	-	0/0/0/0	0/0/0/0
4	SO4	L	303	-	-	0/0/0/0	0/0/0/0
4	SO4	L	304	-	-	0/0/0/0	0/0/0/0
4	SO4	L	305	-	-	0/0/0/0	0/0/0/0
7	1PE	L	306	-	-	0/13/13/13	0/0/0/0
5	GOL	L	307	-	-	0/4/4/4	0/0/0/0
4	SO4	N	601	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	H	304	1PE	1	0
7	J	301	1PE	2	0
4	K	303	SO4	1	0
5	K	304	GOL	1	0
4	L	304	SO4	1	0

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, 95^{th} 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%) 70 73	21, 37, 59, 105	0
1	L	212/214 (99%)	-0.10	2 (0%) 85 88	19, 36, 56, 74	0
2	H	207/221 (93%)	0.02	5 (2%) 62 66	22, 39, 72, 108	0
2	J	207/221 (93%)	0.20	14 (6%) 20 23	23, 45, 85, 111	0
3	M	194/201 (96%)	1.54	53 (27%) 1 1	50, 86, 128, 178	0
3	N	192/201 (95%)	1.21	40 (20%) 1 1	51, 81, 112, 129	0
All	All	1225/1272 (96%)	0.44	118 (9%) 10 11	19, 46, 106, 178	0

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	N	485	LEU	10.5
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	5.0
3	M	337	ASN	5.0
3	N	484	ALA	4.8
3	M	315	GLY	4.7
3	N	319	GLY	4.4
2	H	1	GLN	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	4.2
3	M	417	VAL	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	M	324	SER	4.0
3	N	323	ASP	4.0
3	M	484	ALA	4.0
3	N	315	GLY	3.9
3	M	323	ASP	3.9
3	N	415	ALA	3.9
3	M	495	GLU	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	325	LEU	3.7
3	N	310	LYS	3.7
3	N	311	LYS	3.7
3	M	383	ILE	3.5
3	M	500	VAL	3.5
3	N	324	SER	3.5
3	N	458	GLY	3.5
3	M	339	THR	3.4
3	M	322	LYS	3.4
1	K	212	GLY	3.3
3	M	410	GLY	3.3
3	M	483	HIS	3.2
3	N	460	SER	3.2
2	J	190	VAL	3.2
2	H	192	SER	3.2
3	M	353	ARG	3.1
3	N	337	ASN	3.1
3	N	463	LYS	3.0
3	M	461	GLY	3.0
3	M	416	VAL	3.0
3	N	497	ARG	3.0
3	M	333	LYS	3.0
3	N	317	GLY	2.9
3	M	311	LYS	2.9
3	M	482	CYS	2.9
3	M	490	GLY	2.9
3	M	373	THR	2.9
2	J	198	GLN	2.9
3	M	497	ARG	2.8
3	M	459	THR	2.8
2	J	77	LYS	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	M	335	PHE	2.8
3	M	313	CYS	2.8
3	N	320	GLU	2.7
3	N	416	VAL	2.7
2	J	1	GLN	2.7
3	N	500	VAL	2.7
3	N	501	SER	2.7
3	M	1503	HIS	2.7
3	N	321	PHE	2.7
1	K	188	LYS	2.6
3	N	439	ILE	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	336	LYS	2.5
2	J	26	GLY	2.5
3	N	483	HIS	2.5
3	M	439	ILE	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	2.5
2	J	76	SER	2.4
3	N	322	LYS	2.4
1	K	187	GLU	2.4
3	M	481	VAL	2.4
3	M	359	HIS	2.4
3	N	424	LEU	2.4
2	J	141	THR	2.3
3	N	375	LYS	2.3
3	N	486	CYS	2.3
3	M	358	THR	2.3
3	M	317	GLY	2.3
3	M	328	ASP	2.3
1	L	190	LYS	2.2
2	J	44	GLY	2.2
1	L	56	THR	2.2
2	H	191	PRO	2.2
3	M	415	ALA	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	N	329	ALA	2.2
3	N	459	THR	2.2
3	N	368	LEU	2.1
3	M	479	GLY	2.1
2	H	26	GLY	2.1
3	M	347	ILE	2.1
3	N	383	ILE	2.1
3	M	427	ARG	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 carbohydrates 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. 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, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
4	SO4	N	601	5/5	0.87	0.51	5.65	97,97,99,100	0
5	GOL	K	305	6/6	0.84	0.26	3.44	55,57,59,62	0
5	GOL	H	305	6/6	0.86	0.26	2.96	51,54,57,60	0
7	1PE	L	306	16/16	0.84	0.24	2.78	50,59,67,68	0
6	EDO	K	306	4/4	0.88	0.20	1.18	41,43,47,47	0
7	1PE	J	301	16/16	0.89	0.18	0.54	44,54,68,69	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
7	1PE	H	304	16/16	0.92	0.17	0.47	34,49,56,60	0
5	GOL	K	304	6/6	0.93	0.14	-0.19	48,53,56,57	0
4	SO4	K	303	5/5	0.94	0.18	-0.44	74,79,80,81	0
6	EDO	H	306	4/4	0.94	0.17	-0.50	46,47,48,51	0
4	SO4	L	305	5/5	0.94	0.15	-0.63	68,71,76,77	0
4	SO4	H	302	5/5	0.91	0.25	-	92,94,96,98	0
4	SO4	L	302	5/5	0.87	0.47	-	92,93,96,96	0
4	SO4	K	301	5/5	0.97	0.13	-	66,68,73,74	0
4	SO4	H	303	5/5	0.89	0.30	-	87,90,94,96	0
6	EDO	J	302	4/4	0.95	0.11	-	47,49,52,56	0
5	GOL	L	307	6/6	0.87	0.18	-	44,56,57,57	0
4	SO4	L	303	5/5	0.81	0.47	-	109,111,111,113	0
4	SO4	L	301	5/5	0.87	0.38	-	89,91,97,97	0
4	SO4	H	301	5/5	0.83	0.45	-	89,93,96,97	0
4	SO4	L	304	5/5	0.95	0.12	-	69,72,77,79	0
4	SO4	K	302	5/5	0.85	0.41	-	94,97,98,103	0

6.5 Other polymers (i)

There are no such residues in this entry.