



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 05:17 pm BST

PDB ID : 5SX4
Title : Crystal Structure of panitumumab in complex with epidermal growth factor receptor domain 3.
Authors : Sickmier, E.A.; Kurzeja, R.J.M.; Michelsen, K.; Mukta, V.; Yang, E.; Tasker, A.S.
Deposited on : 2016-08-09
Resolution : 2.80 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 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	:	2.11
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)	:	2.11

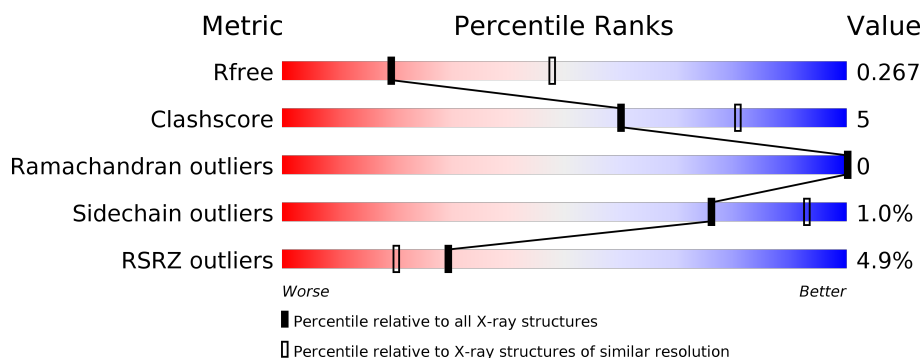
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	I	214	<div> <div>90%</div> <div>9%</div> </div>
1	L	214	<div> <div>91%</div> <div>8%</div> </div>
2	H	221	<div> <div>3%</div> <div>85%</div> <div>10%</div> <div>5%</div> </div>
2	J	221	<div> <div>4%</div> <div>81%</div> <div>10%</div> <div>7%</div> </div>
3	M	201	<div> <div>12%</div> <div>82%</div> <div>13%</div> <div>5%</div> </div>
3	N	201	<div> <div>9%</div> <div>78%</div> <div>14%</div> <div>7%</div> </div>

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	L	304	-	-	-	X

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 9504 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	I	213	Total	C	N	O	S	0	0	0
			1637	1025	273	334	5			
1	L	213	Total	C	N	O	S	0	0	0
			1637	1025	273	334	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	J	205	Total	C	N	O	S	0	0	0
			1544	979	252	307	6			
2	H	210	Total	C	N	O	S	0	0	0
			1578	997	257	318	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	191	Total	C	N	O	S	0	0	0
			1469	922	259	280	8			
3	N	186	Total	C	N	O	S	0	0	0
			1440	905	254	273	8			

There are 24 discrepancies between the modelled and reference sequences:

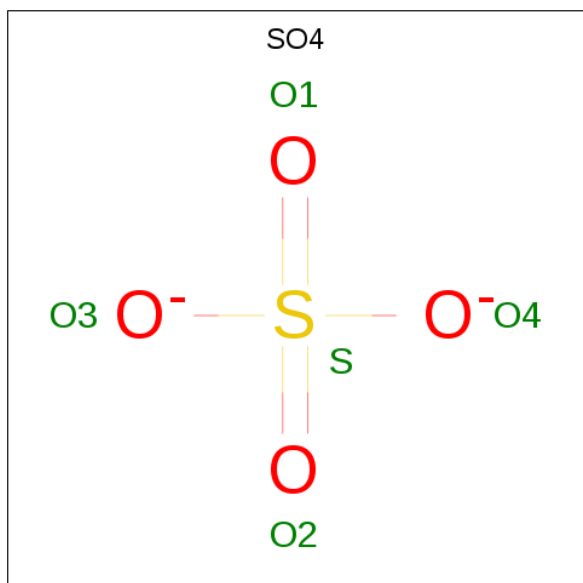
Chain	Residue	Modelled	Actual	Comment	Reference
M	307	LEU	-	expression tag	UNP P00533
M	308	GLU	-	expression tag	UNP P00533
M	309	GLU	-	expression tag	UNP P00533
M	310	LYS	-	expression tag	UNP P00533
M	328	ASP	ASN	conflict	UNP P00533
M	420	ASP	ASN	conflict	UNP P00533
M	502	HIS	-	expression tag	UNP P00533
M	503	HIS	-	expression tag	UNP P00533

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
M	504	HIS	-	expression tag	UNP P00533
M	505	HIS	-	expression tag	UNP P00533
M	506	HIS	-	expression tag	UNP P00533
M	507	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	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	I	1	Total O S 5 4 1	0	0
4	I	1	Total O S 5 4 1	0	0
4	I	1	Total O S 5 4 1	0	0

Continued on next page...

Continued from previous page...

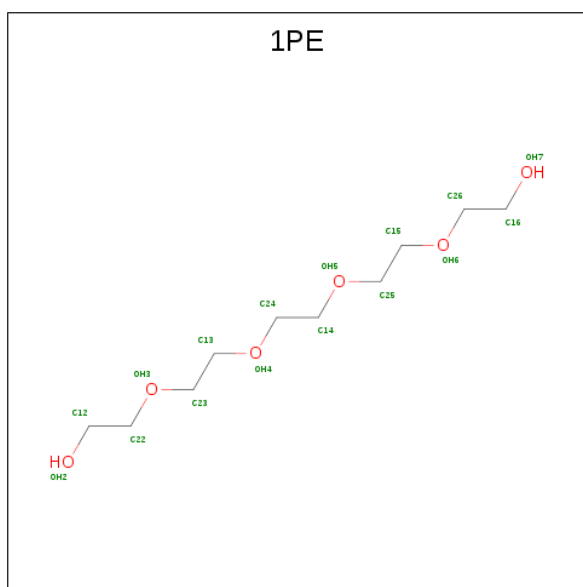
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	L	1	Total	O	S	0	0
			5	4	1		
4	L	1	Total	O	S	0	0
			5	4	1		
4	L	1	Total	O	S	0	0
			5	4	1		
4	L	1	Total	O	S	0	0
			5	4	1		
4	N	1	Total	O	S	0	0
			5	4	1		

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



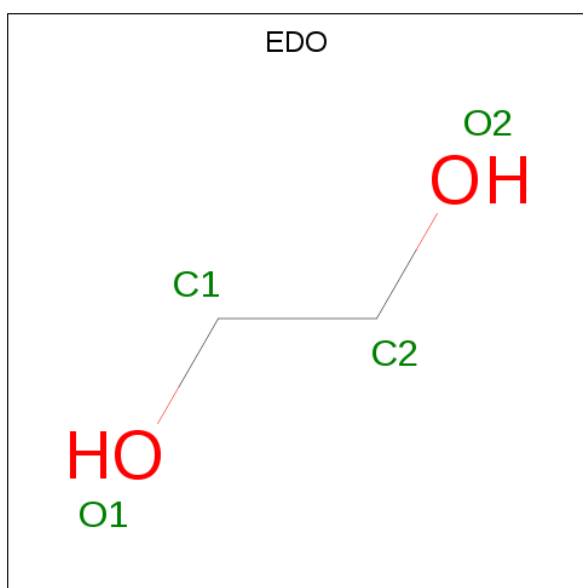
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	I	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



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

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	H	1	Total	C	O	0	0
			4	2	2		

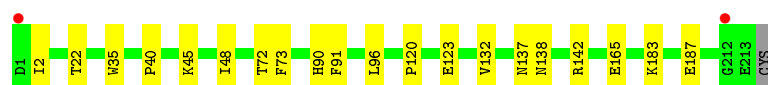
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	I	36	Total 36	O 36	0	0
8	J	16	Total 16	O 16	0	0
8	L	25	Total 25	O 25	0	0
8	H	25	Total 25	O 25	0	0
8	M	10	Total 10	O 10	0	0
8	N	5	Total 5	O 5	0	0

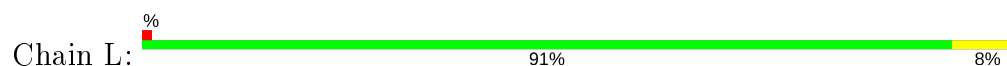
3 Residue-property plots [i](#)

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

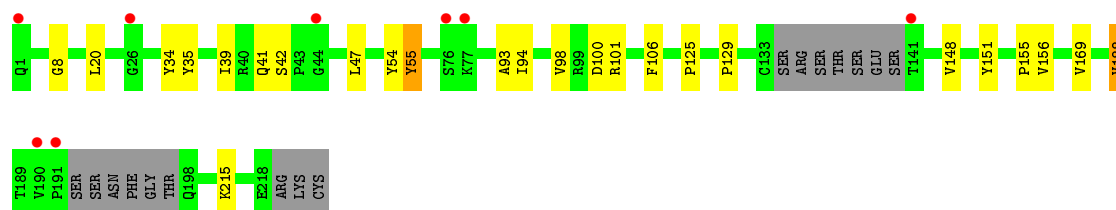
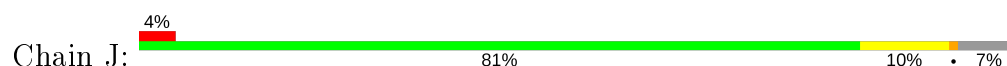
- Molecule 1: Panitumumab Fab Light Chain



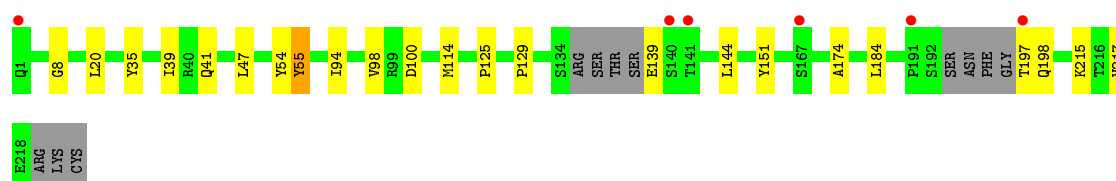
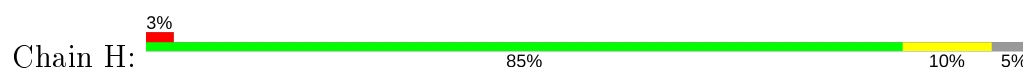
- Molecule 1: Panitumumab Fab Light Chain




- Molecule 2: Panitumumab Fab Heavy Chain

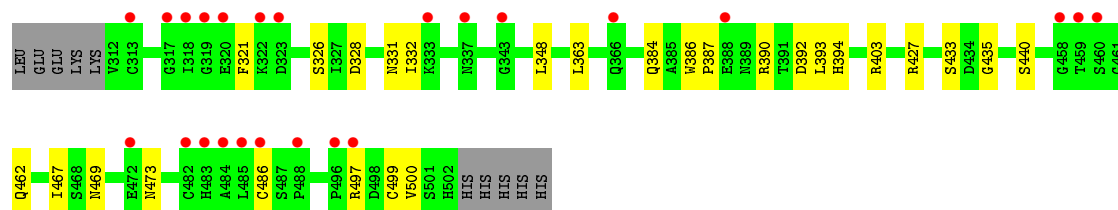


- Molecule 2: Panitumumab Fab Heavy Chain




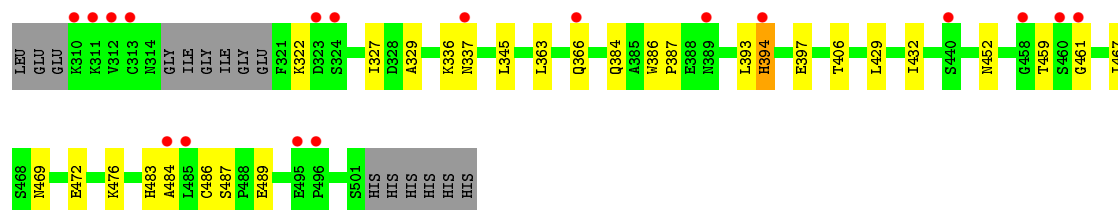
- Molecule 3: Epidermal growth factor receptor

Chain M: 



• Molecule 3: Epidermal growth factor receptor

Chain N: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.27Å 113.18Å 232.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.60 – 2.80 29.60 – 2.78	Depositor EDS
% Data completeness (in resolution range)	88.2 (29.60-2.80) 88.2 (29.60-2.78)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.64 (at 2.76Å)	Xtriage
Refinement program	PHENIX dev_2356	Depositor
R, R_{free}	0.223 , 0.266 0.223 , 0.267	Depositor DCC
R_{free} test set	1974 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	35.5	Xtriage
Anisotropy	0.194	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 43.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	9504	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.70 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.4295e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: 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	I	0.25	0/1673	0.45	0/2272
1	L	0.25	0/1673	0.44	0/2272
2	H	0.25	0/1615	0.46	0/2207
2	J	0.24	0/1581	0.46	0/2161
3	M	0.24	0/1498	0.45	0/2027
3	N	0.24	0/1467	0.44	0/1982
All	All	0.24	0/9507	0.45	0/12921

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	I	1637	0	1579	12	0
1	L	1637	0	1579	11	0
2	H	1578	0	1543	13	0
2	J	1544	0	1513	14	0
3	M	1469	0	1455	19	0
3	N	1440	0	1436	18	0
4	I	15	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	L	20	0	0	1	0
4	N	5	0	0	0	0
5	I	6	0	8	0	0
6	H	16	0	22	3	0
6	J	16	0	22	2	0
7	H	4	0	6	0	0
8	H	25	0	0	0	0
8	I	36	0	0	2	0
8	J	16	0	0	0	0
8	L	25	0	0	1	0
8	M	10	0	0	0	0
8	N	5	0	0	1	0
All	All	9504	0	9163	85	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 5.

All (85) 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)
2:J:55:TYR:OH	3:M:384:GLN:NE2	2.21	0.73
2:H:114:MET:HB2	6:H:301:1PE:H241	1.70	0.72
1:L:40:PRO:HB3	1:L:165:GLU:HG3	1.80	0.62
3:N:483:HIS:HD2	3:N:484:ALA:H	1.48	0.60
1:L:142:ARG:NH1	8:L:401:HOH:O	2.35	0.60
3:M:332:ILE:HD12	3:M:363:LEU:HD23	1.85	0.59
3:N:327:ILE:HD11	3:N:345:LEU:HD22	1.84	0.59
1:I:183:LYS:NZ	1:I:187:GLU:OE2	2.32	0.59
2:J:155:PRO:HB3	6:J:301:1PE:H251	1.83	0.59
1:I:22:THR:HG22	1:I:72:THR:HG22	1.86	0.58
1:L:123:GLU:N	1:L:123:GLU:OE1	2.34	0.58
3:M:386:TRP:CG	3:M:387:PRO:HD2	2.40	0.57
2:H:55:TYR:OH	3:N:384:GLN:NE2	2.38	0.56
1:I:40:PRO:HB3	1:I:165:GLU:HG3	1.87	0.56
1:L:210:ASN:HB2	1:L:213:GLU:HG2	1.88	0.55
1:L:211:ARG:NH2	4:L:304:SO4:O2	2.40	0.54
1:I:137:ASN:ND2	1:I:138:ASN:OD1	2.41	0.54
1:L:137:ASN:ND2	1:L:138:ASN:OD1	2.41	0.53
1:I:123:GLU:OE1	1:I:123:GLU:N	2.37	0.53
3:N:483:HIS:CD2	3:N:484:ALA:H	2.26	0.52
2:H:125:PRO:HB3	2:H:151:TYR:HB3	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:472:GLU:HG2	3:N:476:LYS:HE3	1.91	0.52
3:M:435:GLY:O	3:M:462:GLN:NE2	2.39	0.51
3:M:390:ARG:HH12	3:M:394:HIS:CE1	2.29	0.51
2:H:94:ILE:HD13	6:H:301:1PE:H262	1.93	0.51
3:M:386:TRP:CD2	3:M:387:PRO:HD2	2.46	0.50
3:M:467:ILE:O	3:M:469:ASN:ND2	2.45	0.50
2:J:35:TYR:N	2:J:100:ASP:O	2.32	0.50
1:L:120:PRO:HD3	1:L:132:VAL:HG22	1.94	0.49
1:I:91:PHE:HA	1:I:96:LEU:HD22	1.93	0.49
3:N:394:HIS:HB2	3:N:397:GLU:HB3	1.94	0.49
3:M:326:SER:HB2	3:M:348:LEU:HG	1.93	0.49
3:M:390:ARG:HH22	3:M:394:HIS:CE1	2.31	0.49
2:H:94:ILE:HD11	6:H:301:1PE:H221	1.95	0.48
2:J:129:PRO:HD3	2:J:215:LYS:HE3	1.95	0.48
1:I:2:ILE:HD12	1:I:90:HIS:CE1	2.50	0.47
1:I:45:LYS:NZ	8:I:404:HOH:O	2.47	0.47
2:J:125:PRO:HB3	2:J:151:TYR:HB3	1.96	0.47
1:L:35:TRP:CE2	1:L:73:PHE:HB2	2.50	0.46
3:N:336:LYS:HG3	3:N:337:ASN:HD22	1.80	0.46
3:N:337:ASN:ND2	8:N:701:HOH:O	2.49	0.46
3:M:386:TRP:CE2	3:M:393:LEU:HD23	2.49	0.46
1:I:35:TRP:CE2	1:I:73:PHE:HB2	2.51	0.46
3:N:366:GLN:OE1	3:N:366:GLN:N	2.49	0.46
2:J:8:GLY:HA3	2:J:20:LEU:HD23	1.97	0.45
2:H:129:PRO:HD3	2:H:215:LYS:HE3	1.99	0.45
2:J:98:VAL:HG11	2:J:106:PHE:HB3	1.99	0.45
2:H:41:GLN:HB2	2:H:47:LEU:HD23	1.98	0.45
3:M:486:CYS:HB2	3:M:499:CYS:HB3	1.93	0.45
3:N:386:TRP:CG	3:N:387:PRO:HD2	2.52	0.45
2:H:35:TYR:N	2:H:100:ASP:O	2.28	0.44
2:J:34:TYR:HA	2:J:101:ARG:HA	1.99	0.44
3:N:467:ILE:O	3:N:469:ASN:ND2	2.50	0.44
3:N:452:ASN:N	3:N:489:GLU:O	2.48	0.44
2:J:94:ILE:HG21	6:J:301:1PE:H132	1.98	0.44
3:M:427:ARG:HD2	3:M:497:ARG:HG2	1.99	0.44
3:N:386:TRP:CE2	3:N:393:LEU:HD23	2.53	0.44
2:H:174:ALA:HA	2:H:184:LEU:HB3	2.00	0.44
2:H:8:GLY:HA3	2:H:20:LEU:HD23	2.00	0.44
2:J:39:ILE:HD12	2:J:98:VAL:HG21	2.00	0.44
3:N:329:ALA:HB2	3:N:363:LEU:HA	1.99	0.44
3:M:321:PHE:HE2	3:M:331:ASN:HB2	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:429:LEU:HD21	3:N:432:ILE:HD11	1.99	0.43
3:M:403:ARG:HA	3:M:433:SER:HB2	2.00	0.43
3:M:440:SER:HA	3:M:467:ILE:O	2.19	0.43
2:J:169:VAL:HG22	2:J:188:VAL:HG13	2.01	0.43
3:M:321:PHE:CE2	3:M:331:ASN:HB2	2.53	0.43
1:L:91:PHE:HA	1:L:96:LEU:HD22	2.01	0.42
1:L:105:GLU:OE1	1:L:173:TYR:OH	2.34	0.42
3:M:328:ASP:HA	3:M:363:LEU:HD11	2.01	0.42
4:I:302:SO4:O2	3:M:473:ASN:ND2	2.53	0.42
3:N:322:LYS:HD2	3:N:322:LYS:HA	1.79	0.42
2:J:148:VAL:HG11	2:J:156:VAL:HG11	2.01	0.42
1:L:189:HIS:O	1:L:211:ARG:NH1	2.49	0.42
3:N:459:THR:HG22	3:N:461:GLY:H	1.85	0.42
1:I:120:PRO:HD3	1:I:132:VAL:HG22	2.01	0.42
1:I:142:ARG:NH2	8:I:407:HOH:O	2.54	0.41
2:J:41:GLN:HB2	2:J:47:LEU:HD23	2.01	0.41
2:H:39:ILE:HD12	2:H:98:VAL:HG21	2.03	0.41
1:I:35:TRP:HB2	1:I:48:ILE:HB	2.03	0.41
3:M:386:TRP:NE1	3:M:392:ASP:O	2.54	0.41
3:N:487:SER:C	3:N:489:GLU:H	2.24	0.41
2:H:139:GLU:OE2	2:H:139:GLU:N	2.54	0.41
2:H:144:LEU:HB2	2:H:217:VAL:HG11	2.03	0.40
2:J:42:SER:HB3	2:J:93:ALA:HB2	2.03	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	I	211/214 (99%)	206 (98%)	5 (2%)	0	100	100
1	L	211/214 (99%)	204 (97%)	7 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	204/221 (92%)	198 (97%)	6 (3%)	0	100	100
2	J	199/221 (90%)	192 (96%)	7 (4%)	0	100	100
3	M	189/201 (94%)	177 (94%)	12 (6%)	0	100	100
3	N	182/201 (90%)	173 (95%)	9 (5%)	0	100	100
All	All	1196/1272 (94%)	1150 (96%)	46 (4%)	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	I	187/188 (100%)	187 (100%)	0	100	100
1	L	187/188 (100%)	187 (100%)	0	100	100
2	H	183/193 (95%)	179 (98%)	4 (2%)	52	83
2	J	178/193 (92%)	175 (98%)	3 (2%)	60	87
3	M	166/176 (94%)	165 (99%)	1 (1%)	86	96
3	N	164/176 (93%)	161 (98%)	3 (2%)	59	86
All	All	1065/1114 (96%)	1054 (99%)	11 (1%)	76	93

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	J	54	TYR
2	J	55	TYR
2	J	188	VAL
2	H	54	TYR
2	H	55	TYR
2	H	197	THR
2	H	198	GLN
3	M	500	VAL
3	N	394	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	N	406	THR
3	N	486	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	I	53	ASN
1	I	137	ASN
1	L	53	ASN
1	L	137	ASN
2	H	60	ASN
2	H	170	HIS
3	M	337	ASN
3	M	384	GLN
3	M	473	ASN
3	M	480	GLN
3	N	337	ASN
3	N	384	GLN
3	N	394	HIS
3	N	483	HIS

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 ⓘ

12 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	L	302	-	4,4,4	0.14	0	6,6,6	0.06	0
4	SO4	L	303	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	I	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	0.06	0
6	1PE	J	301	-	15,15,15	0.60	0	14,14,14	0.23	0
5	GOL	I	304	-	5,5,5	0.37	0	5,5,5	0.26	0
4	SO4	I	301	-	4,4,4	0.14	0	6,6,6	0.04	0
4	SO4	N	601	-	4,4,4	0.14	0	6,6,6	0.05	0
7	EDO	H	302	-	3,3,3	0.46	0	2,2,2	0.36	0
4	SO4	I	302	-	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	0.06	0
6	1PE	H	301	-	15,15,15	0.59	0	14,14,14	0.23	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	EDO	H	302	-	-	0/1/1/1	-
5	GOL	I	304	-	-	2/4/4/4	-
6	1PE	J	301	-	-	7/13/13/13	-
6	1PE	H	301	-	-	7/13/13/13	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	I	304	GOL	O1-C1-C2-C3
6	H	301	1PE	OH4-C13-C23-OH3
6	H	301	1PE	OH5-C14-C24-OH4
6	J	301	1PE	OH7-C16-C26-OH6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	J	301	1PE	OH6-C15-C25-OH5
5	I	304	GOL	O1-C1-C2-O2
6	J	301	1PE	C14-C24-OH4-C13
6	J	301	1PE	C25-C15-OH6-C26
6	H	301	1PE	OH7-C16-C26-OH6
6	H	301	1PE	C23-C13-OH4-C24
6	J	301	1PE	C13-C23-OH3-C22
6	H	301	1PE	C25-C15-OH6-C26
6	J	301	1PE	OH5-C14-C24-OH4
6	H	301	1PE	C24-C14-OH5-C25
6	J	301	1PE	OH4-C13-C23-OH3
6	H	301	1PE	OH6-C15-C25-OH5

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	304	SO4	1	0
6	J	301	1PE	2	0
4	I	302	SO4	1	0
6	H	301	1PE	3	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	I	213/214 (99%)	-0.35	2 (0%) 84 80	20, 37, 59, 73	0
1	L	213/214 (99%)	-0.35	2 (0%) 84 80	21, 38, 58, 73	0
2	H	210/221 (95%)	-0.23	6 (2%) 51 41	21, 41, 77, 97	0
2	J	205/221 (92%)	-0.17	8 (3%) 39 29	24, 43, 75, 97	0
3	M	191/201 (95%)	0.89	24 (12%) 3 2	55, 86, 111, 131	0
3	N	186/201 (92%)	0.60	18 (9%) 7 4	50, 78, 104, 119	0
All	All	1218/1272 (95%)	0.04	60 (4%) 29 20	20, 47, 99, 131	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	M	319	GLY	7.3
3	M	337	ASN	6.2
3	M	318	ILE	5.5
3	N	323	ASP	5.3
3	N	485	LEU	4.9
3	M	320	GLU	4.6
1	L	213	GLU	4.3
3	N	460	SER	4.2
3	N	484	ALA	4.1
3	N	389	ASN	4.0
3	M	485	LEU	4.0
3	M	488	PRO	3.7
3	N	495	GLU	3.6
3	M	496	PRO	3.6
2	J	1	GLN	3.6
3	M	333	LYS	3.5
3	M	484	ALA	3.5
3	M	460	SER	3.5
3	M	459	THR	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	J	77	LYS	3.3
2	J	141	THR	3.3
2	J	191	PRO	3.2
3	M	313	CYS	3.1
2	H	1	GLN	3.1
1	I	212	GLY	3.1
3	N	324	SER	3.0
3	N	366	GLN	2.9
3	M	497	ARG	2.9
3	M	483	HIS	2.9
2	H	197	THR	2.9
3	N	496	PRO	2.8
3	M	322	LYS	2.8
3	M	323	ASP	2.8
3	N	337	ASN	2.7
2	J	190	VAL	2.7
1	L	56	THR	2.6
3	N	312	VAL	2.6
1	I	1	ASP	2.5
2	H	140	SER	2.5
3	N	310	LYS	2.4
2	J	44	GLY	2.3
3	N	313	CYS	2.3
2	H	141	THR	2.3
3	M	486	CYS	2.3
3	M	458	GLY	2.3
3	N	440	SER	2.3
2	H	191	PRO	2.3
3	N	311	LYS	2.2
3	M	343	GLY	2.2
3	N	394	HIS	2.2
3	N	461	GLY	2.2
3	N	458	GLY	2.2
3	M	482	CYS	2.2
3	M	366	GLN	2.1
2	J	26	GLY	2.1
3	M	317	GLY	2.1
2	H	167	SER	2.1
2	J	76	SER	2.1
3	M	388	GLU	2.1
3	M	472	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. 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(\AA^2)	Q<0.9
4	SO4	L	304	5/5	0.71	0.46	109,109,117,118	0
4	SO4	N	601	5/5	0.89	0.40	88,97,105,106	0
4	SO4	L	301	5/5	0.90	0.21	73,77,87,93	0
5	GOL	I	304	6/6	0.91	0.14	50,56,62,69	0
4	SO4	I	302	5/5	0.92	0.24	73,83,91,101	0
4	SO4	I	303	5/5	0.93	0.32	100,104,112,113	0
6	1PE	J	301	16/16	0.94	0.18	34,54,67,74	0
7	EDO	H	302	4/4	0.94	0.20	34,40,47,56	0
6	1PE	H	301	16/16	0.94	0.15	20,42,54,62	0
4	SO4	I	301	5/5	0.96	0.16	73,81,85,85	0
4	SO4	L	303	5/5	0.96	0.13	78,93,98,101	0
4	SO4	L	302	5/5	0.98	0.15	49,70,74,81	0

6.5 Other polymers [i](#)

There are no such residues in this entry.