



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 08:04 AM UTC

PDB ID : 5LSP / pdb_00005lsp
Title : 107_A07 Fab in complex with fragment of the Met receptor
Authors : DiCara, D.; Chirgadze, D.Y.; Pope, A.; Karatt-Vellatt, A.; Winter, A.; van den Heuvel, J.; Gherardi, E.; McCafferty, J.
Deposited on : 2016-09-05
Resolution : 2.60 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

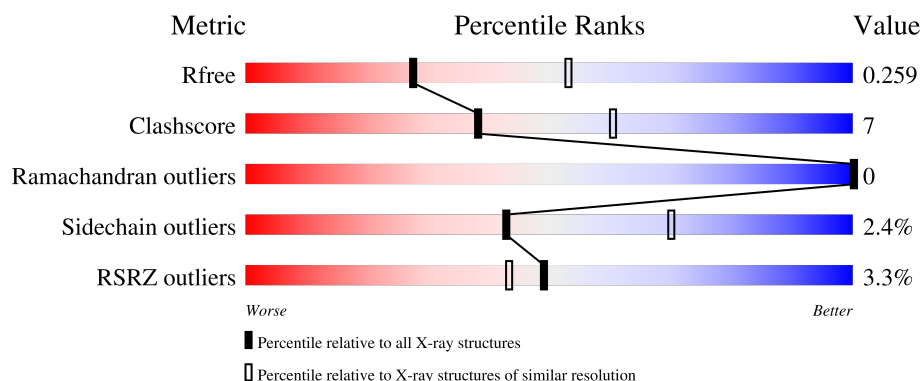
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

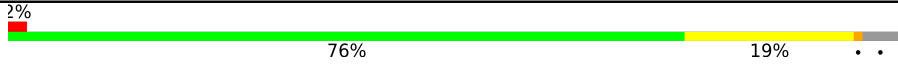
The reported resolution of this entry is 2.60 Å.

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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	A	231	
1	P	231	
2	H	223	
2	S	223	
3	L	216	

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Mol	Chain	Length	Quality of chain
3	T	216	% 81%16%..
4	X	14	21%43%21%36%
4	Y	14	43%64%7%29%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10159 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 Hepatocyte growth factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	222	Total	C	N	O	S	0	0	0
			1705	1070	294	324	17			
1	P	222	Total	C	N	O	S	0	0	0
			1705	1070	294	324	17			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	744	HIS	-	expression tag	UNP P08581
A	745	HIS	-	expression tag	UNP P08581
A	746	HIS	-	expression tag	UNP P08581
A	747	HIS	-	expression tag	UNP P08581
A	748	HIS	-	expression tag	UNP P08581
A	749	HIS	-	expression tag	UNP P08581
P	744	HIS	-	expression tag	UNP P08581
P	745	HIS	-	expression tag	UNP P08581
P	746	HIS	-	expression tag	UNP P08581
P	747	HIS	-	expression tag	UNP P08581
P	748	HIS	-	expression tag	UNP P08581
P	749	HIS	-	expression tag	UNP P08581

- Molecule 2 is a protein called 107_A07 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	216	Total	C	N	O	S	0	0	0
			1628	1036	260	322	10			
2	S	216	Total	C	N	O	S	0	0	0
			1628	1036	260	322	10			

- Molecule 3 is a protein called 107_A07 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	212	Total	C	N	O	S	0	0	0
			1625	1014	274	332	5			
3	T	212	Total	C	N	O	S	0	0	0
			1625	1014	274	332	5			

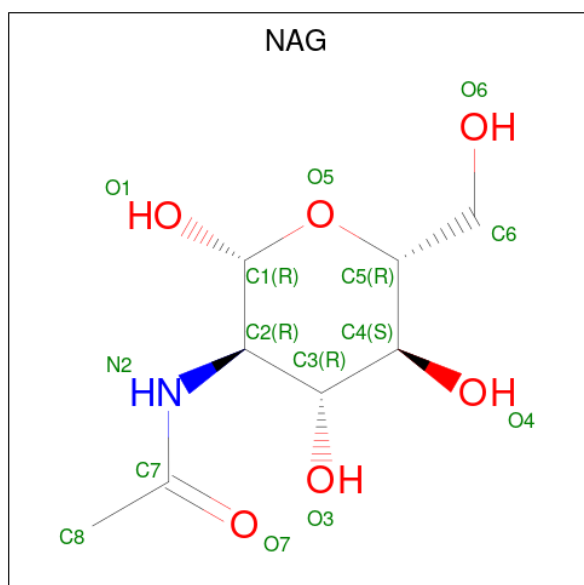
- Molecule 4 is a protein called Hepatocyte growth factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	X	9	Total	C	N	O	S	0	0	0
			59	35	9	14	1			
4	Y	10	Total	C	N	O	S	0	0	0
			68	41	11	15	1			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	22	GLU	-	expression tag	UNP P08581
X	23	THR	-	expression tag	UNP P08581
X	24	ARG	-	expression tag	UNP P08581
Y	22	GLU	-	expression tag	UNP P08581
Y	23	THR	-	expression tag	UNP P08581
Y	24	ARG	-	expression tag	UNP P08581

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	P	1	Total	C	N	O	0	0
			14	8	1	5		

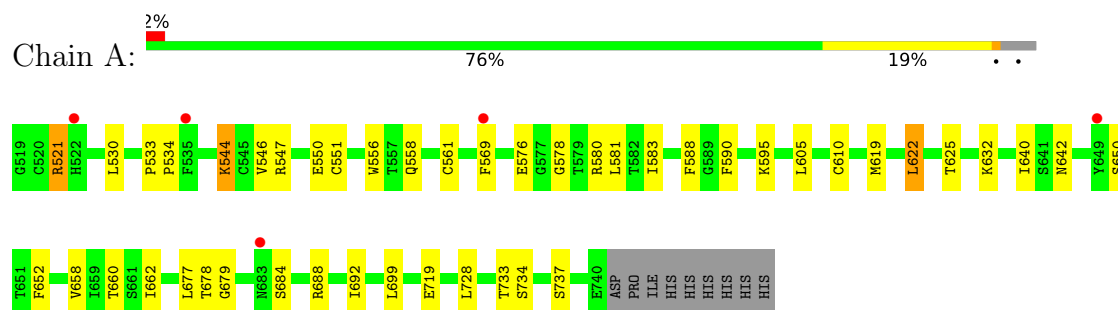
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	18	Total	O	0	0
			18	18		
6	H	21	Total	O	0	0
			21	21		
6	L	22	Total	O	0	0
			22	22		
6	P	4	Total	O	0	0
			4	4		
6	S	13	Total	O	0	0
			13	13		
6	T	10	Total	O	0	0
			10	10		

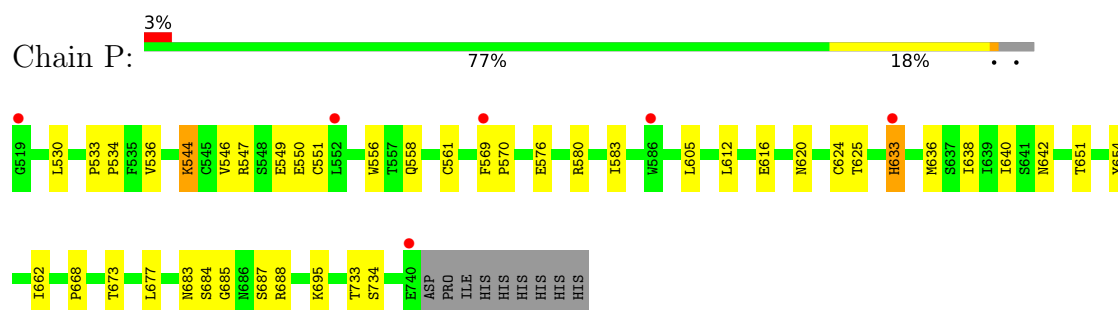
3 Residue-property plots

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.

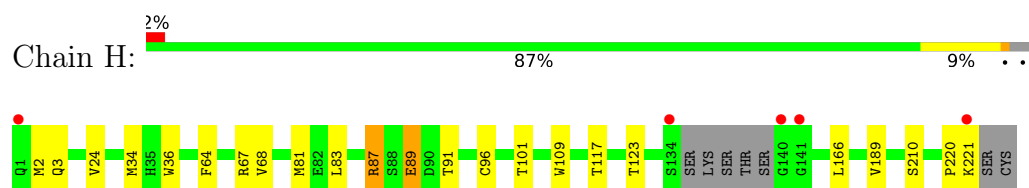
- Molecule 1: Hepatocyte growth factor receptor



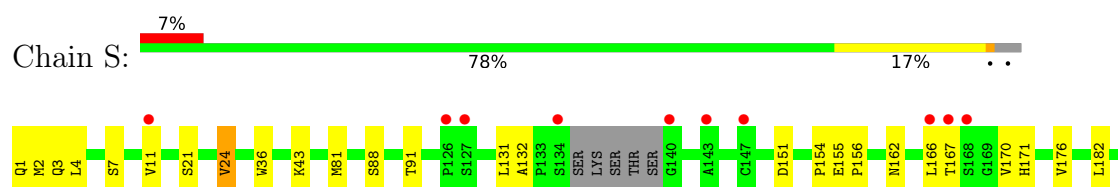
- Molecule 1: Hepatocyte growth factor receptor



- Molecule 2: 107_A07 Fab heavy chain



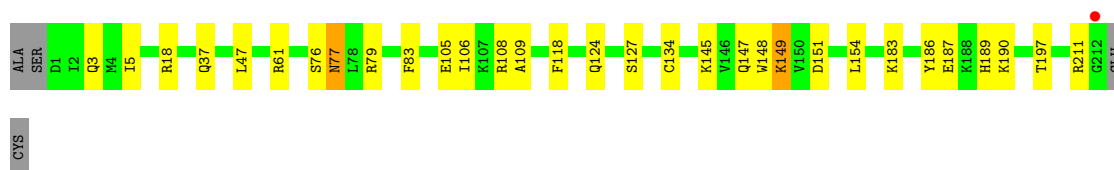
- Molecule 2: 107_A07 Fab heavy chain





- Molecule 3: 107_A07 Fab light chain

Chain L: 84% 13% ..



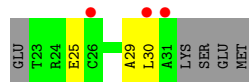
- Molecule 3: 107_A07 Fab light chain

Chain T: 81% 16% ..



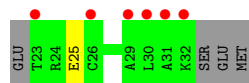
- Molecule 4: Hepatocyte growth factor receptor

Chain X: 21% 43% 21% 36%



- Molecule 4: Hepatocyte growth factor receptor

Chain Y: 43% 64% 7% 29%



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.88Å 82.28Å 267.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.94 – 2.60 48.94 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.8 (48.94-2.60) 98.8 (48.94-2.60)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.215 , 0.257 0.220 , 0.259	Depositor DCC
R_{free} test set	2000 reflections (4.09%)	wwPDB-VP
Wilson B-factor (Å ²)	50.0	Xtriage
Anisotropy	0.533	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 37.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10159	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% 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: NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.34	0/1742	0.82	1/2360 (0.0%)
1	P	0.32	0/1742	0.79	0/2360
2	H	0.34	0/1671	0.72	0/2283
2	S	0.42	0/1671	0.87	5/2283 (0.2%)
3	L	0.31	0/1659	0.77	2/2252 (0.1%)
3	T	0.34	0/1659	0.78	4/2252 (0.2%)
4	X	0.66	0/58	1.06	0/78
4	Y	0.32	0/67	0.89	0/89
All	All	0.35	0/10269	0.80	12/13957 (0.1%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	118	PHE	CA-C-N	6.49	124.40	119.66
3	L	118	PHE	C-N-CA	6.49	124.40	119.66
2	S	132	ALA	CA-C-N	6.37	126.34	120.03
2	S	132	ALA	C-N-CA	6.37	126.34	120.03
3	T	118	PHE	CA-C-N	6.11	124.12	119.66
3	T	118	PHE	C-N-CA	6.11	124.12	119.66
2	S	218	VAL	N-CA-C	5.65	116.00	107.80
2	S	193	SER	N-CA-C	-5.64	105.23	111.71
1	A	650	SER	N-CA-C	5.61	118.48	110.68
2	S	202	ILE	CA-CB-CG1	5.58	119.88	110.40
3	T	112	ALA	CA-C-N	5.15	125.05	119.85
3	T	112	ALA	C-N-CA	5.15	125.05	119.85

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	A	1705	0	1676	32	0
1	P	1705	0	1676	25	0
2	H	1628	0	1579	20	0
2	S	1628	0	1579	30	0
3	L	1625	0	1570	19	0
3	T	1625	0	1570	19	0
4	X	59	0	47	5	0
4	Y	68	0	60	1	0
5	A	14	0	13	0	0
5	P	14	0	13	0	0
6	A	18	0	0	0	0
6	H	21	0	0	0	0
6	L	22	0	0	1	0
6	P	4	0	0	0	0
6	S	13	0	0	1	0
6	T	10	0	0	0	0
All	All	10159	0	9783	137	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 7.

All (137) 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)
1:A:684:SER:O	1:A:688:ARG:NH1	2.15	0.80
1:P:636:MET:HE1	1:P:654:TYR:HD2	1.56	0.70
1:A:569:PHE:HD2	4:X:30:LEU:HD13	1.60	0.67
1:A:595:LYS:NZ	2:H:101:THR:O	2.27	0.67
3:L:187:GLU:O	3:L:211:ARG:NH2	2.28	0.66
2:H:3:GLN:NE2	2:S:3:GLN:HE22	1.93	0.66
3:T:206:THR:O	3:T:207:LYS:HD3	1.96	0.64
2:S:196:LEU:HD11	2:S:199:GLN:O	1.98	0.64
1:A:580:ARG:HG2	1:A:625:THR:HG22	1.80	0.64
2:S:212:THR:O	2:S:213:LYS:HD3	1.98	0.63
1:A:530:LEU:HD22	1:A:558:GLN:HA	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:620:ASN:HB2	4:Y:25:GLU:OE1	1.98	0.62
2:S:207:HIS:CD2	2:S:209:PRO:HD2	2.35	0.61
1:P:580:ARG:NH2	1:P:616:GLU:OE2	2.33	0.61
1:P:636:MET:HE1	1:P:654:TYR:CD2	2.36	0.60
3:L:183:LYS:O	3:L:187:GLU:HG3	2.00	0.60
3:L:145:LYS:HG2	3:L:197:THR:HB	1.82	0.60
2:S:170:VAL:C	2:S:171:HIS:HD1	2.12	0.57
1:A:561:CYS:O	1:A:642:ASN:ND2	2.33	0.57
3:T:183:LYS:O	3:T:187:GLU:HG3	2.05	0.57
1:P:547:ARG:NH1	1:P:549:GLU:OE2	2.37	0.56
2:H:91:THR:HG23	2:H:117:THR:HA	1.87	0.56
1:A:544:LYS:HG2	1:A:546:VAL:HG23	1.87	0.56
2:S:11:VAL:HB	2:S:154:PRO:HG3	1.88	0.56
2:H:220:PRO:O	2:H:221:LYS:HB2	2.06	0.56
1:P:683:ASN:HA	1:P:688:ARG:HE	1.71	0.56
2:S:212:THR:C	2:S:213:LYS:HD3	2.31	0.55
2:S:216:LYS:HE2	3:T:123:GLU:OE1	2.06	0.55
2:S:162:ASN:HD22	2:S:166:LEU:HD13	1.71	0.55
1:A:521:ARG:NH1	1:A:521:ARG:HG2	2.20	0.55
3:L:151:ASP:OD1	3:L:190:LYS:HB3	2.06	0.54
2:S:36:TRP:CE2	2:S:81:MET:HB2	2.42	0.54
1:A:733:THR:OG1	1:A:734:SER:N	2.33	0.54
2:S:196:LEU:HD13	2:S:201:TYR:HE2	1.72	0.54
2:S:131:LEU:HD22	3:T:118:PHE:HB3	1.91	0.53
2:H:166:LEU:HD21	2:H:189:VAL:HG21	1.89	0.53
2:S:196:LEU:HA	2:S:198:THR:H	1.72	0.53
3:L:37:GLN:HB2	3:L:47:LEU:HD11	1.90	0.53
2:H:109:TRP:CD1	2:S:1:GLN:HE21	2.27	0.53
3:L:3:GLN:NE2	3:L:5:ILE:HD11	2.24	0.52
2:H:36:TRP:CE2	2:H:81:MET:HB2	2.44	0.52
1:P:583:ILE:HD13	1:P:640:ILE:HD11	1.90	0.52
3:T:22:THR:HG22	3:T:72:THR:HG22	1.92	0.52
1:A:660:THR:N	1:A:678:THR:O	2.42	0.52
1:A:569:PHE:HD2	4:X:30:LEU:CD1	2.23	0.52
1:P:544:LYS:HB3	1:P:546:VAL:HG23	1.91	0.52
1:P:551:CYS:SG	1:P:556:TRP:HB2	2.50	0.52
1:A:546:VAL:HG11	1:A:550:GLU:HB2	1.91	0.52
1:P:662:ILE:HG22	1:P:677:LEU:HD22	1.91	0.52
3:L:189:HIS:O	3:L:211:ARG:HD3	2.09	0.51
2:S:176:VAL:HG11	3:T:160:GLN:HB3	1.93	0.51
3:T:37:GLN:HB2	3:T:47:LEU:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:202:ILE:HG13	2:S:217:LYS:HD3	1.91	0.50
2:S:151:ASP:HB3	2:S:182:LEU:HD13	1.93	0.50
1:P:633:HIS:HB3	1:P:636:MET:HE2	1.92	0.50
1:A:688:ARG:HB2	1:A:699:LEU:HD11	1.94	0.50
1:P:733:THR:OG1	1:P:734:SER:N	2.40	0.50
1:P:569:PHE:CD1	1:P:570:PRO:HA	2.47	0.49
3:L:18:ARG:HG2	3:L:76:SER:HA	1.93	0.49
3:T:120:PRO:HD3	3:T:132:VAL:HG22	1.93	0.49
1:P:576:GLU:OE1	1:P:576:GLU:N	2.43	0.48
1:P:580:ARG:HG2	1:P:625:THR:HG22	1.95	0.48
2:H:109:TRP:HB3	2:S:1:GLN:NE2	2.28	0.48
3:T:158:ASN:HD22	3:T:181:LEU:HD21	1.78	0.48
2:H:2:MET:C	2:H:3:GLN:HG2	2.37	0.48
1:P:561:CYS:O	1:P:642:ASN:ND2	2.41	0.48
2:S:170:VAL:O	2:S:171:HIS:ND1	2.40	0.47
2:H:64:PHE:O	2:H:68:VAL:HG12	2.14	0.47
3:L:124:GLN:O	3:L:127:SER:OG	2.22	0.47
1:A:588:PHE:CD2	1:A:622:LEU:HD13	2.50	0.47
2:H:3:GLN:HE21	2:H:3:GLN:HA	1.79	0.47
1:P:530:LEU:HD22	1:P:558:GLN:HA	1.96	0.47
2:S:215:ASP:OD2	6:S:301:HOH:O	2.20	0.47
3:L:108:ARG:HG3	3:L:109:ALA:O	2.14	0.47
1:A:521:ARG:HG2	1:A:521:ARG:HH11	1.80	0.47
3:T:108:ARG:HE	3:T:172:THR:HG22	1.80	0.46
2:H:3:GLN:HE22	2:S:3:GLN:NE2	2.12	0.46
3:L:105:GLU:OE2	6:L:301:HOH:O	2.20	0.46
2:S:162:ASN:HD22	2:S:166:LEU:CD1	2.28	0.46
3:T:39:LYS:HD3	3:T:84:ALA:HB2	1.96	0.46
3:T:146:VAL:HG11	3:T:177:SER:HB2	1.97	0.46
1:A:569:PHE:CD2	4:X:30:LEU:HD13	2.46	0.46
3:L:79:ARG:HD3	3:L:79:ARG:HA	1.72	0.46
3:L:147:GLN:NE2	3:L:154:LEU:HD11	2.31	0.46
3:T:149:LYS:HB2	3:T:193:ALA:HB3	1.97	0.45
1:A:662:ILE:HG22	1:A:677:LEU:HD22	1.97	0.45
1:A:605:LEU:HB2	1:A:610:CYS:SG	2.57	0.45
2:H:89:GLU:H	2:H:89:GLU:HG3	1.35	0.45
3:T:114:SER:HB2	3:T:137:ASN:HB3	1.98	0.45
3:L:3:GLN:HE21	3:L:5:ILE:HD11	1.80	0.45
1:P:687:SER:HA	1:P:688:ARG:NH1	2.32	0.45
3:T:148:TRP:HB2	3:T:155:GLN:HB2	1.99	0.45
1:P:612:LEU:HD23	1:P:624:CYS:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:578:GLY:HA3	1:A:728:LEU:HG	1.99	0.45
3:L:61:ARG:HD2	3:L:77:ASN:HB3	2.00	0.44
1:P:605:LEU:HD13	1:P:638:ILE:HG12	2.00	0.44
1:P:546:VAL:CG1	1:P:550:GLU:HG3	2.48	0.44
2:H:3:GLN:NE2	2:S:3:GLN:NE2	2.64	0.43
1:P:533:PRO:HA	1:P:534:PRO:HD3	1.89	0.43
2:S:11:VAL:HG13	2:S:11:VAL:O	2.19	0.43
1:A:658:VAL:O	1:A:679:GLY:HA3	2.18	0.43
1:A:546:VAL:CG1	1:A:550:GLU:HB2	2.49	0.43
1:A:583:ILE:HG21	1:A:640:ILE:HD11	2.01	0.42
3:T:140:TYR:CG	3:T:141:PRO:HA	2.54	0.42
1:A:544:LYS:NZ	1:A:544:LYS:HB3	2.34	0.42
2:H:3:GLN:HE22	2:S:3:GLN:HE22	1.64	0.42
2:H:34:MET:HE3	2:H:34:MET:HB3	1.89	0.42
3:L:134:CYS:HB2	3:L:148:TRP:CH2	2.54	0.42
3:L:149:LYS:HE2	3:L:149:LYS:HB2	1.72	0.42
3:T:108:ARG:NE	3:T:172:THR:HG22	2.34	0.42
1:A:533:PRO:HA	1:A:534:PRO:HD3	1.85	0.42
1:A:581:LEU:HD21	1:A:652:PHE:CE1	2.55	0.42
1:A:551:CYS:SG	1:A:556:TRP:HB2	2.60	0.41
1:A:619:MET:HE3	1:A:619:MET:HB3	1.88	0.41
2:H:67:ARG:HD3	2:H:87:ARG:NH1	2.35	0.41
1:A:590:PHE:HB2	1:A:642:ASN:O	2.20	0.41
2:H:123:THR:HG22	2:H:210:SER:HB3	2.01	0.41
3:L:83:PHE:CZ	3:L:106:ILE:HG12	2.55	0.41
1:P:662:ILE:HG12	1:P:734:SER:HB2	2.02	0.41
2:S:7:SER:HB3	2:S:21:SER:OG	2.20	0.41
3:T:122:ASP:O	3:T:126:LYS:HG2	2.20	0.41
1:A:719:GLU:HG3	1:A:737:SER:HB2	2.03	0.41
1:P:684:SER:HA	1:P:685:GLY:HA2	1.87	0.41
2:S:2:MET:N	2:S:2:MET:SD	2.92	0.41
2:H:34:MET:HE1	2:H:96:CYS:HB2	2.02	0.41
2:H:83:LEU:HD23	2:H:83:LEU:HA	1.89	0.41
3:L:186:TYR:O	3:L:211:ARG:HD2	2.21	0.41
2:S:88:SER:O	2:S:91:THR:HG22	2.20	0.41
2:S:155:GLU:CB	2:S:156:PRO:HA	2.51	0.41
3:T:158:ASN:O	3:T:179:LEU:HD12	2.21	0.41
4:X:25:GLU:O	4:X:29:ALA:N	2.52	0.41
4:X:30:LEU:HD23	4:X:30:LEU:HA	1.86	0.41
1:A:576:GLU:OE1	1:A:576:GLU:N	2.53	0.40
1:P:668:PRO:HD2	1:P:673:THR:OG1	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:4:LEU:HD22	2:S:24:VAL:HG12	2.02	0.40
1:A:546:VAL:HG12	1:A:547:ARG:N	2.36	0.40
1:A:632:LYS:HE2	1:A:632:LYS:HB2	1.91	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	A	220/231 (95%)	213 (97%)	7 (3%)	0	100	100
1	P	220/231 (95%)	210 (96%)	10 (4%)	0	100	100
2	H	212/223 (95%)	205 (97%)	7 (3%)	0	100	100
2	S	212/223 (95%)	202 (95%)	10 (5%)	0	100	100
3	L	210/216 (97%)	203 (97%)	7 (3%)	0	100	100
3	T	210/216 (97%)	203 (97%)	7 (3%)	0	100	100
4	X	7/14 (50%)	7 (100%)	0	0	100	100
4	Y	8/14 (57%)	8 (100%)	0	0	100	100
All	All	1299/1368 (95%)	1251 (96%)	48 (4%)	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	A	196/205 (96%)	192 (98%)	4 (2%)	48	74
1	P	196/205 (96%)	191 (97%)	5 (3%)	40	68
2	H	181/189 (96%)	178 (98%)	3 (2%)	53	78
2	S	181/189 (96%)	172 (95%)	9 (5%)	22	46
3	L	184/187 (98%)	182 (99%)	2 (1%)	65	84
3	T	184/187 (98%)	180 (98%)	4 (2%)	45	72
4	X	5/12 (42%)	5 (100%)	0	100	100
4	Y	6/12 (50%)	6 (100%)	0	100	100
All	All	1133/1186 (96%)	1106 (98%)	27 (2%)	43	70

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	521	ARG
1	A	544	LYS
1	A	622	LEU
1	A	692	ILE
2	H	24	VAL
2	H	87	ARG
2	H	89	GLU
3	L	77	ASN
3	L	149	LYS
1	P	536	VAL
1	P	544	LYS
1	P	633	HIS
1	P	651	THR
1	P	695	LYS
2	S	24	VAL
2	S	43	LYS
2	S	167	THR
2	S	194	SER
2	S	199	GLN
2	S	202	ILE
2	S	216	LYS
2	S	219	GLU
2	S	221	LYS
3	T	33	LEU
3	T	107	LYS
3	T	126	LYS
3	T	138	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	633	HIS
1	A	644	HIS
2	H	1	GLN
2	H	3	GLN
3	L	3	GLN
3	L	77	ASN
1	P	559	GLN
1	P	633	HIS
1	P	704	ASN
3	T	189	HIS
3	T	210	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	$\# Z > 2$
5	NAG	P	1000	1	14,14,15	0.57	0	17,19,21	0.91	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	A	1000	1	14,14,15	0.32	0	17,19,21	0.75	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	P	1000	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1000	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	P	1000	NAG	C1-O5-C5	3.02	116.23	112.19
5	A	1000	NAG	C1-O5-C5	2.09	114.98	112.19

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1000	NAG	O5-C5-C6-O6
5	P	1000	NAG	O5-C5-C6-O6
5	P	1000	NAG	C4-C5-C6-O6
5	A	1000	NAG	C4-C5-C6-O6
5	A	1000	NAG	C8-C7-N2-C2
5	A	1000	NAG	O7-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	222/231 (96%)	0.18	5 (2%) 61 55	37, 48, 79, 95	0
1	P	222/231 (96%)	0.47	6 (2%) 56 50	45, 65, 86, 97	0
2	H	216/223 (96%)	0.08	5 (2%) 61 55	33, 47, 70, 85	0
2	S	216/223 (96%)	0.64	15 (6%) 23 18	44, 72, 102, 120	0
3	L	212/216 (98%)	0.10	1 (0%) 87 85	32, 49, 78, 84	0
3	T	212/216 (98%)	0.34	2 (0%) 81 78	40, 56, 92, 105	0
4	X	9/14 (64%)	1.63	3 (33%) 1 1	85, 91, 96, 101	0
4	Y	10/14 (71%)	1.87	6 (60%) 0 0	88, 96, 100, 101	0
All	All	1319/1368 (96%)	0.32	43 (3%) 49 43	32, 56, 93, 120	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	134	SER	5.2
4	X	30	LEU	4.7
2	S	214	VAL	3.1
2	H	1	GLN	3.0
3	L	212	GLY	3.0
1	P	586	TRP	3.0
2	S	168	SER	2.9
1	A	649	TYR	2.8
2	S	127	SER	2.8
1	P	552	LEU	2.8
2	S	140	GLY	2.8
1	P	519	GLY	2.6
2	S	221	LYS	2.6
2	S	194	SER	2.6
4	Y	32	LYS	2.5
2	S	126	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
4	X	26	CYS	2.5
2	S	11	VAL	2.5
1	A	569	PHE	2.4
4	X	31	ALA	2.4
2	H	141	GLY	2.4
2	S	166	LEU	2.4
2	H	221	LYS	2.4
3	T	212	GLY	2.3
2	S	147	CYS	2.3
2	S	218	VAL	2.3
1	P	569	PHE	2.3
4	Y	23	THR	2.3
2	S	134	SER	2.3
2	S	220	PRO	2.2
4	Y	30	LEU	2.2
1	P	740	GLU	2.2
2	H	140	GLY	2.2
2	S	143	ALA	2.2
2	S	167	THR	2.1
1	P	633	HIS	2.1
4	Y	31	ALA	2.1
1	A	683	ASN	2.1
1	A	535	PHE	2.1
3	T	211	ARG	2.0
4	Y	29	ALA	2.0
1	A	522	HIS	2.0
4	Y	26	CYS	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($\text{\AA}^2$)	Q<0.9
5	NAG	P	1000	14/15	0.63	0.18	86,96,104,104	0
5	NAG	A	1000	14/15	0.84	0.11	73,77,82,82	0

6.5 Other polymers [i](#)

There are no such residues in this entry.