



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:01 AM UTC

PDB ID : 6WIT / pdb_00006wit
Title : Crystal structure of NHP D15.SD7 Fab in complex with 16055 V1V2 1FD6 scaffold
Authors : Liban, T.; Aljedani, S.; Rodarte, J.; Pancera, M.
Deposited on : 2020-04-10
Resolution : 2.79 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

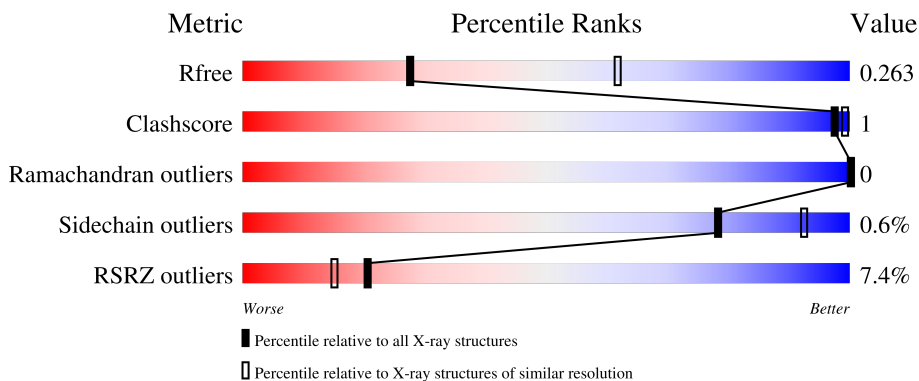
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.79 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.



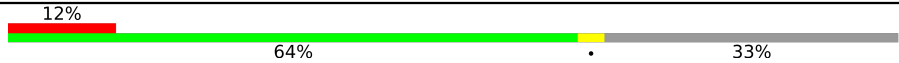
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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 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	232	 4% 95%
1	H	232	 2% 94%
2	B	213	 17% 98%
2	L	213	 % 99%
3	C	129	 10% 77% 21%

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Mol	Chain	Length	Quality of chain
3	I	129	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into three segments: a red segment on the left labeled '12%', a green segment in the middle labeled '64%', and a grey segment on the right labeled '33%'. A small yellow dot is located at the end of the green segment.</p>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16065 atoms, of which 7861 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 NHP GN1-SD7 Fab Heavy Chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	226	Total 3339	C 1075	H 1634	N 284	O 337	S 9	0	0	0
1	H	223	Total 3344	C 1076	H 1639	N 286	O 335	S 8	0	0	0

- Molecule 2 is a protein called NHP GN1-SD7 Fab Light Chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	B	210	Total 2946	C 948	H 1412	N 260	O 322	S 4	0	0	0
2	L	213	Total 3125	C 991	H 1526	N 273	O 331	S 4	0	0	0

- Molecule 3 is a protein called 16055 V1V2 1FD6 Scaffold.

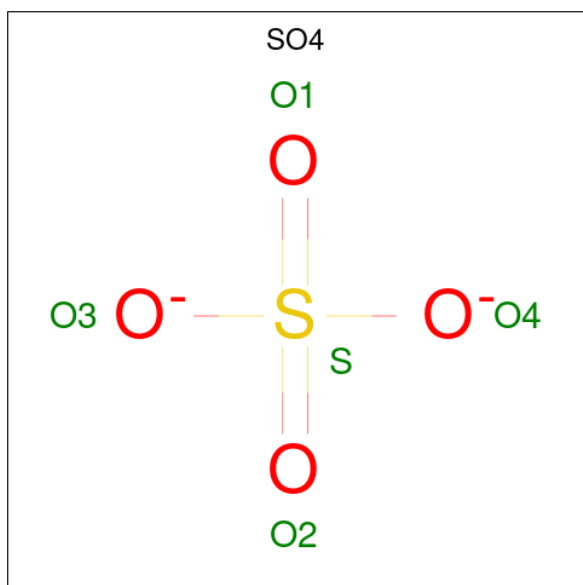
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
3	C	102	Total 1577	C 505	H 772	N 132	O 163	S 5	0	0	0
3	I	87	Total 1401	C 446	H 692	N 120	O 139	S 4	0	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	H	N			O
4	C	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
4	I	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
4	I	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
4	I	1	Total	C	H	N	O	0	0
			27	8	13	1	5		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

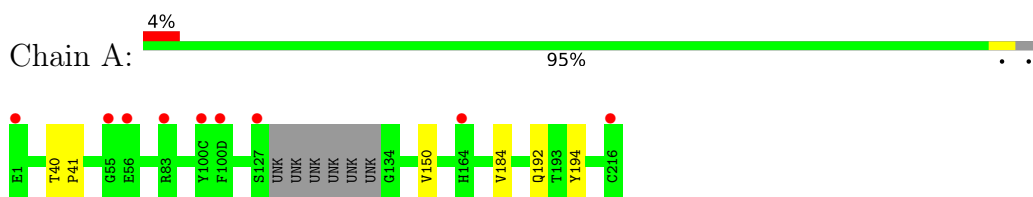
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	26	Total H O 78 52 26	0	0
6	B	1	Total H O 3 2 1	0	0
6	C	1	Total H O 3 2 1	0	0
6	H	24	Total H O 66 42 24	0	0
6	L	14	Total H O 40 26 14	0	0
6	I	5	Total H O 15 10 5	0	0

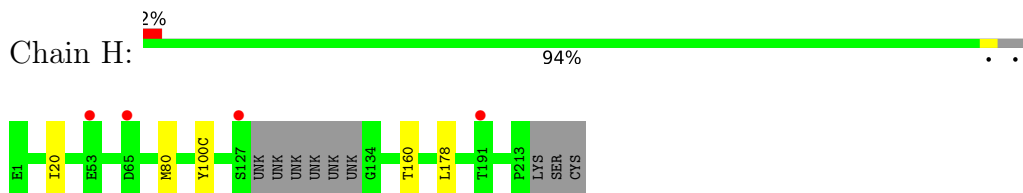
3 Residue-property plots [i](#)

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.

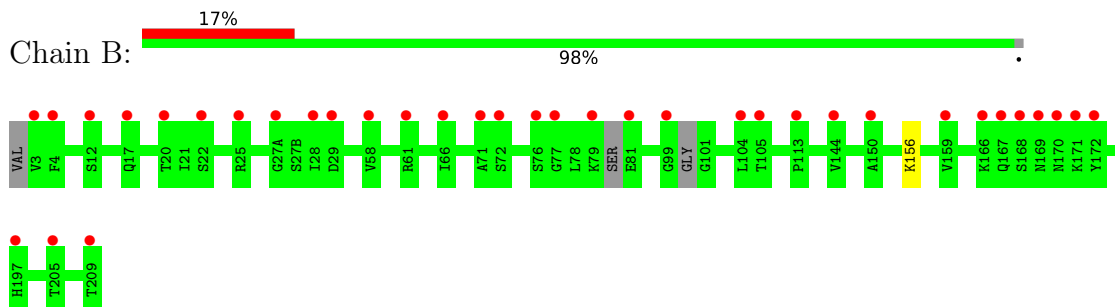
- Molecule 1: NHP GN1-SD7 Fab Heavy Chain



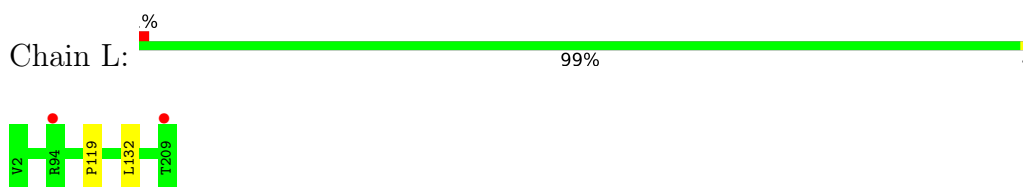
- Molecule 1: NHP GN1-SD7 Fab Heavy Chain



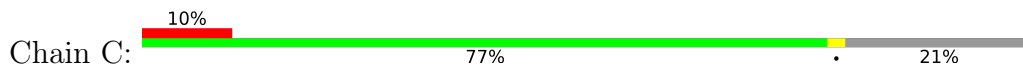
- Molecule 2: NHP GN1-SD7 Fab Light Chain

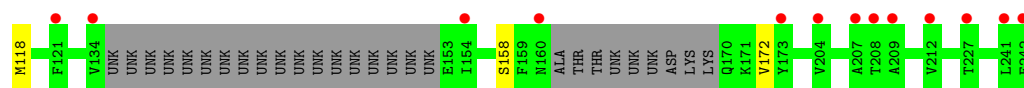


- Molecule 2: NHP GN1-SD7 Fab Light Chain

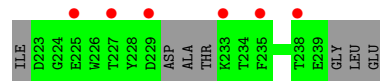
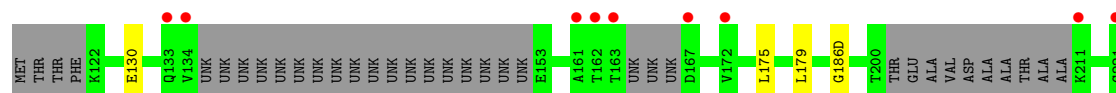


- Molecule 3: 16055 V1V2 1FD6 Scaffold





- Molecule 3: 16055 V1V2 1FD6 Scaffold



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.41Å 89.81Å 172.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.48 – 2.79 48.48 – 2.79	Depositor EDS
% Data completeness (in resolution range)	95.8 (48.48-2.79) 91.0 (48.48-2.79)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 2.81Å)	Xtrriage
Refinement program	PHENIX (1.17.1_3660: ???)	Depositor
R, R_{free}	0.224 , 0.284 (Not available) , 0.263	Depositor DCC
R_{free} test set	2000 reflections (7.10%)	wwPDB-VP
Wilson B-factor (Å ²)	45.2	Xtrriage
Anisotropy	0.083	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 53.9	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	0.90	EDS
Total number of atoms	16065	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtrriage'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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, 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	A	0.21	0/1749	0.42	0/2385
1	H	0.26	0/1750	0.44	0/2385
2	B	0.25	0/1570	0.44	0/2147
2	L	0.25	0/1638	0.43	0/2237
3	C	0.26	0/815	0.47	0/1101
3	I	0.27	0/715	0.47	0/955
All	All	0.25	0/8237	0.44	0/11210

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	A	1705	1634	1633	2	0
1	H	1705	1639	1638	3	0
2	B	1534	1412	1410	0	0
2	L	1599	1526	1526	1	0
3	C	805	772	771	2	0
3	I	709	692	689	3	0
4	C	14	13	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	I	42	39	39	4	0
5	C	5	0	0	0	0
5	H	10	0	0	0	0
5	L	5	0	0	0	0
6	A	26	52	0	0	0
6	B	1	2	0	0	0
6	C	1	2	0	0	0
6	H	24	42	0	0	0
6	I	5	10	0	0	0
6	L	14	26	0	0	0
All	All	8204	7861	7719	12	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 1.

All (12) 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:I:186(D):GLY:HA3	4:I:303:NAG:H82	1.66	0.77
4:I:303:NAG:O7	4:I:303:NAG:O3	2.09	0.69
1:H:100(C):TYR:O	3:I:179:LEU:HD13	2.08	0.53
2:L:119:PRO:HA	2:L:132:LEU:HD23	1.91	0.52
3:C:118:MET:HE2	3:C:118:MET:HA	1.90	0.52
3:C:158:SER:HA	3:C:172:VAL:O	2.13	0.48
1:H:20:ILE:HD11	1:H:80:MET:HE2	1.95	0.47
1:A:40:THR:HG23	1:A:41:PRO:HD2	1.96	0.47
3:I:175:LEU:HD21	4:I:301:NAG:H82	1.98	0.45
1:H:178:LEU:C	1:H:178:LEU:HD12	2.42	0.44
4:I:303:NAG:HO3	4:I:303:NAG:C7	2.26	0.44
1:A:192:GLN:HG2	1:A:194:TYR:CZ	2.56	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	222/232 (96%)	218 (98%)	4 (2%)	0	100	100
1	H	219/232 (94%)	214 (98%)	5 (2%)	0	100	100
2	B	204/213 (96%)	198 (97%)	6 (3%)	0	100	100
2	L	211/213 (99%)	206 (98%)	5 (2%)	0	100	100
3	C	96/129 (74%)	93 (97%)	3 (3%)	0	100	100
3	I	75/129 (58%)	75 (100%)	0	0	100	100
All	All	1027/1148 (90%)	1004 (98%)	23 (2%)	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	190/194 (98%)	188 (99%)	2 (1%)	65	87
1	H	190/194 (98%)	189 (100%)	1 (0%)	81	93
2	B	168/183 (92%)	167 (99%)	1 (1%)	78	92
2	L	182/183 (100%)	182 (100%)	0	100	100
3	C	87/93 (94%)	87 (100%)	0	100	100
3	I	79/93 (85%)	78 (99%)	1 (1%)	61	86
All	All	896/940 (95%)	891 (99%)	5 (1%)	78	92

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

Mol	Chain	Res	Type
1	A	150	VAL
1	A	184	VAL
2	B	156	LYS
1	H	160	THR
3	I	130	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	39	GLN
2	B	38	GLN
2	B	53	GLN
2	B	95(A)	ASN
2	L	53	GLN
3	I	215	GLN
3	I	218	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](#)

8 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	SO4	H	302	-	4,4,4	0.30	0	6,6,6	0.10	0
5	SO4	L	301	-	4,4,4	0.25	0	6,6,6	0.11	0
4	NAG	C	301	3	14,14,15	0.34	0	17,19,21	0.50	0
4	NAG	I	301	3	14,14,15	0.27	0	17,19,21	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	I	302	3	14,14,15	0.23	0	17,19,21	0.41	0
4	NAG	I	303	3	14,14,15	0.37	0	17,19,21	0.53	0
5	SO4	C	302	-	4,4,4	0.26	0	6,6,6	0.06	0
5	SO4	H	301	-	4,4,4	0.26	0	6,6,6	0.14	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	NAG	I	303	3	-	2/6/23/26	0/1/1/1
4	NAG	C	301	3	-	3/6/23/26	0/1/1/1
4	NAG	I	301	3	-	2/6/23/26	0/1/1/1
4	NAG	I	302	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	I	301	NAG	C4-C5-C6-O6
4	I	301	NAG	O5-C5-C6-O6
4	C	301	NAG	O5-C5-C6-O6
4	C	301	NAG	C1-C2-N2-C7
4	I	303	NAG	C1-C2-N2-C7
4	C	301	NAG	C3-C2-N2-C7
4	I	303	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	301	NAG	1	0
4	I	303	NAG	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	226/232 (97%)	0.36	9 (3%) 42 33	32, 55, 88, 115	0
1	H	223/232 (96%)	0.07	4 (1%) 67 58	25, 48, 83, 96	0
2	B	210/213 (98%)	1.18	36 (17%) 4 3	43, 77, 104, 116	0
2	L	213/213 (100%)	0.20	2 (0%) 81 74	26, 54, 86, 103	0
3	C	102/129 (79%)	0.82	13 (12%) 8 6	39, 72, 95, 105	0
3	I	87/129 (67%)	0.79	15 (17%) 4 3	29, 61, 108, 118	0
All	All	1061/1148 (92%)	0.51	79 (7%) 20 15	25, 60, 96, 118	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	170	ASN	6.1
2	B	4	PHE	5.3
2	B	71	ALA	4.9
2	B	79	LYS	4.8
1	A	100(D)	PHE	4.1
1	A	100(C)	TYR	4.0
1	A	1	GLU	3.9
2	B	66	ILE	3.6
2	B	168	SER	3.6
1	A	56	GLU	3.5
3	I	235	PHE	3.5
3	I	172	VAL	3.4
2	B	22	SER	3.3
3	I	238	THR	3.3
2	B	167	GLN	3.3
3	I	225	GLU	3.3
2	B	172	TYR	3.3
2	B	171	LYS	3.1
3	C	204	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
3	I	162	THR	3.0
1	A	55	GLY	3.0
1	H	53	GLU	2.8
2	B	72	SER	2.8
2	B	209	THR	2.8
2	L	94	ARG	2.7
3	C	134	VAL	2.7
3	I	221	GLY	2.7
3	C	209	ALA	2.7
2	L	209	THR	2.7
2	B	197	HIS	2.6
1	A	164	HIS	2.6
2	B	25	ARG	2.6
1	H	65	ASP	2.6
2	B	3	VAL	2.6
3	C	241	LEU	2.5
2	B	61	ARG	2.5
3	C	242	GLU	2.5
2	B	104	LEU	2.5
2	B	105	THR	2.4
3	C	227	THR	2.4
3	C	154	ILE	2.4
2	B	150	ALA	2.4
3	C	173	TYR	2.4
3	I	161	ALA	2.4
2	B	20	THR	2.3
3	I	233	LYS	2.3
2	B	58	VAL	2.3
3	C	208	THR	2.3
1	H	127	SER	2.3
2	B	12	SER	2.3
2	B	29	ASP	2.3
2	B	28	ILE	2.3
2	B	81	GLU	2.3
1	H	191	THR	2.2
2	B	169	ASN	2.2
2	B	27(A)	GLY	2.2
2	B	99	GLY	2.2
1	A	216	CYS	2.2
2	B	17	GLN	2.2
3	I	133	GLN	2.2
3	I	167	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	76	SER	2.2
2	B	159	VAL	2.2
3	I	134	VAL	2.2
3	I	163	THR	2.1
2	B	166	LYS	2.1
1	A	127	SER	2.1
2	B	205	THR	2.1
2	B	113	PRO	2.1
3	C	121	PHE	2.1
2	B	77	GLY	2.1
3	C	212	VAL	2.1
1	A	83	ARG	2.0
3	I	229	ASP	2.0
3	I	211	LYS	2.0
3	I	227	THR	2.0
3	C	160	ASN	2.0
3	C	207	ALA	2.0
2	B	144	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	I	302	14/15	0.68	0.12	53,86,110,116	0
4	NAG	C	301	14/15	0.75	0.12	60,74,106,114	0
4	NAG	I	303	14/15	0.75	0.15	75,101,129,137	0
5	SO4	H	302	5/5	0.86	0.34	35,49,102,106	0
4	NAG	I	301	14/15	0.89	0.10	64,79,109,131	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	SO4	L	301	5/5	0.91	0.14	61,64,75,89	0
5	SO4	C	302	5/5	0.94	0.09	61,67,71,73	0
5	SO4	H	301	5/5	0.94	0.09	42,54,66,70	0

6.5 Other polymers [i](#)

There are no such residues in this entry.