Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 06:28 am BST

PDB ID	:	6OBD
Title	:	Crystal structure of anti-GLD52 Fab complex with human GLD52 peptide mimetic
Authors	:	Wei, R.
Deposited on	:	2019-03-20
Resolution	:	2.20 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:

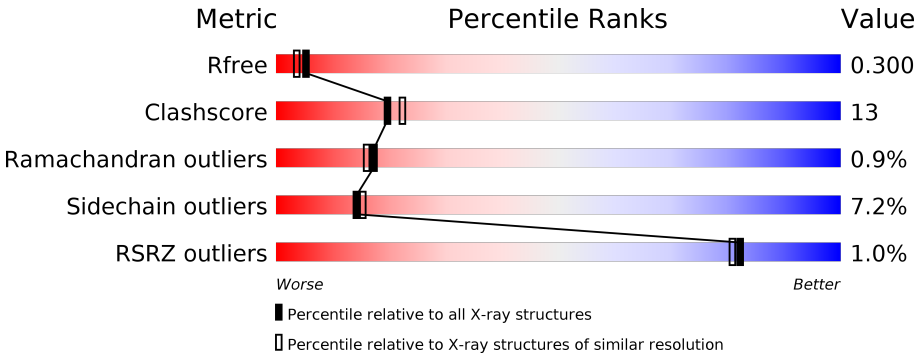
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 <=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	216	80% 16%
1	L	216	75% 23%
2	B	216	78% 16%
2	H	216	2% 72% 23%
3	E	10	30% 60% 10%
3	F	10	20% 40% 20% 40%

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
5	OPE	F	101	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7253 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 anti-GLD52 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	0	0	0
			1659	1041	280	333	5			
1	L	216	Total	C	N	O	S	0	0	0
			1659	1042	280	332	5			

- Molecule 2 is a protein called anti-GLD52 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	211	Total	C	N	O	S	0	0	0
			1591	1006	267	312	6			
2	H	211	Total	C	N	O	S	0	0	0
			1587	1003	266	312	6			

- Molecule 3 is a protein called GLD52 peptide mimetic.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	9	Total	C	N	O	0	0	0
			62	34	10	18			
3	F	10	Total	C	N	O	0	0	0
			70	38	12	20			

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	1	Total	Zn	0	0
			1	1		
4	B	1	Total	Zn	0	0
			1	1		
4	A	1	Total	Zn	0	0
			1	1		
4	L	1	Total	Zn	0	0
			1	1		

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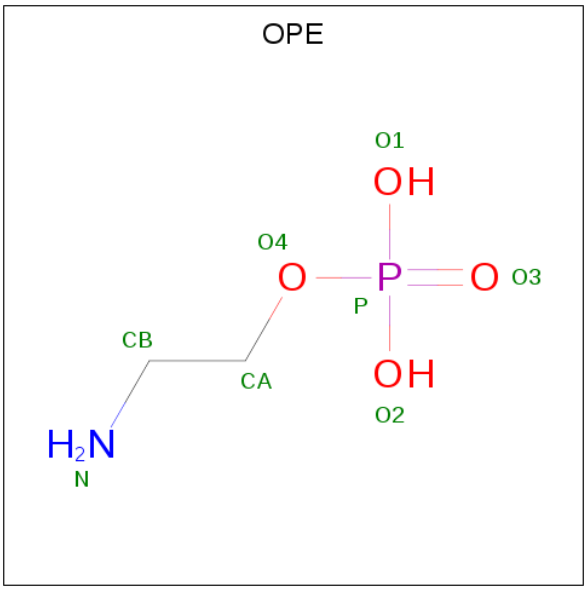
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	1	Total Zn 1 1	0	0

- Molecule 5 is PHOSPHORIC ACID MONO-(2-AMINO-ETHYL) ESTER (three-letter code: OPE) (formula: $C_2H_8NO_4P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	1	Total C N O P 8 2 1 4 1	0	0
5	F	1	Total C N O P 8 2 1 4 1	0	0

- Molecule 6 is water.

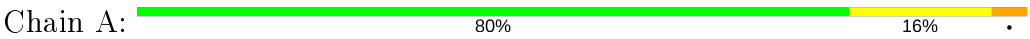
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	166	Total O 166 166	0	0
6	B	169	Total O 169 169	0	0
6	L	130	Total O 130 130	0	0
6	H	123	Total O 123 123	0	0
6	E	6	Total O 6 6	0	0
6	F	10	Total O 10 10	0	0

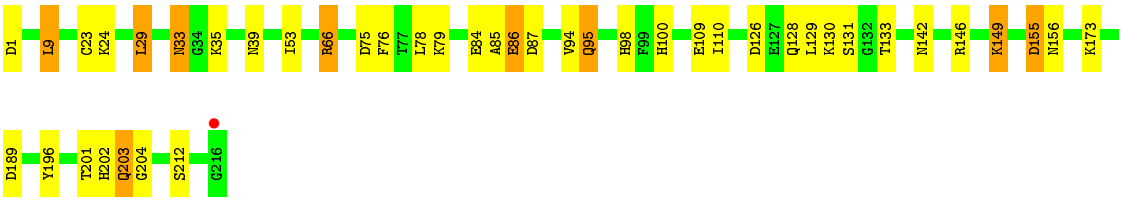
3 Residue-property plots (i)

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: anti-GLD52 Fab light chain

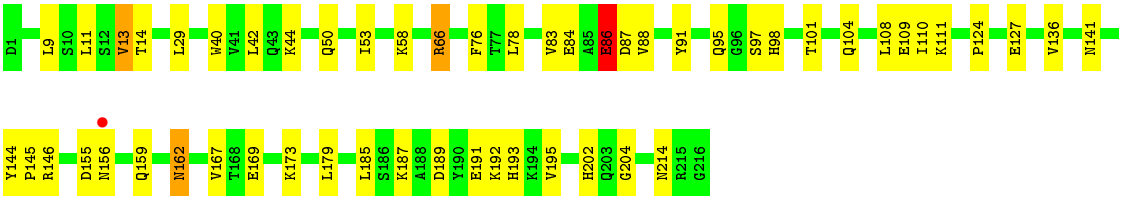
Chain A:





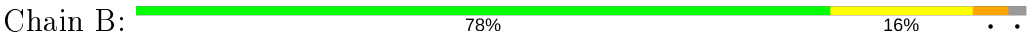
- Molecule 1: anti-GLD52 Fab light chain

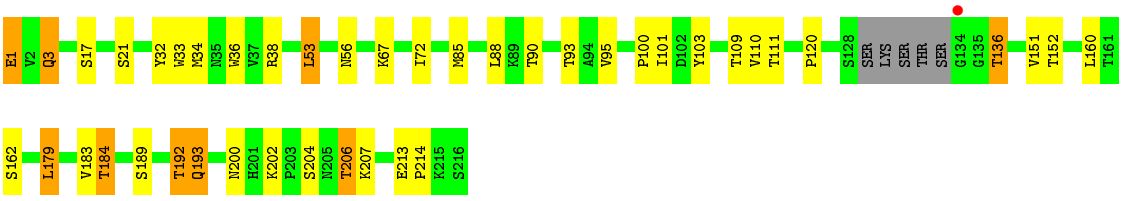
Chain L:



- Molecule 2: anti-GLD52 Fab heavy chain

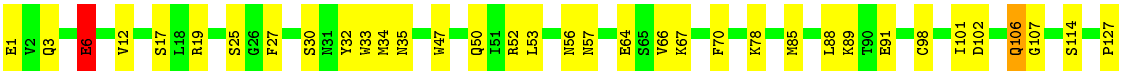
Chain B:

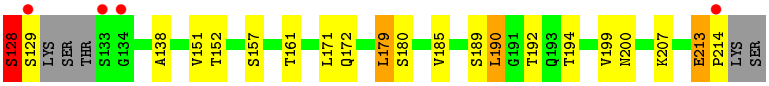




- Molecule 2: anti-GLD52 Fab heavy chain

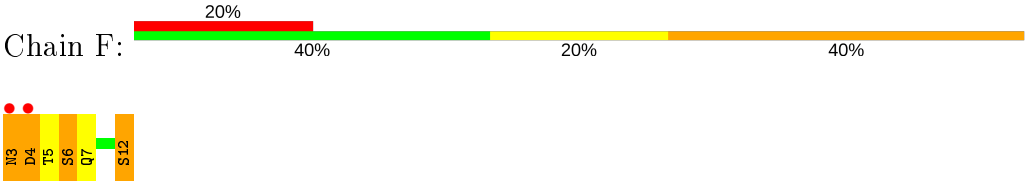
Chain H:





- Molecule 3: GLD52 peptide mimetic

- Molecule 3: GLD52 peptide mimetic



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	54.40Å 131.20Å 133.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.53 – 2.20 30.53 – 2.20	Depositor EDS
% Data completeness (in resolution range)	95.4 (30.53-2.20) 95.5 (30.53-2.20)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.58 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.234 , 0.307 0.230 , 0.300	Depositor DCC
R_{free} test set	2387 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	32.8	Xtriage
Anisotropy	0.191	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 31.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7253	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.42% 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: OPE, ZN

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	0.97	2/1694 (0.1%)	0.89	4/2296 (0.2%)
1	L	0.90	0/1694	0.99	6/2296 (0.3%)
2	B	0.93	1/1631 (0.1%)	0.86	0/2221
2	H	0.94	3/1627 (0.2%)	0.89	1/2218 (0.0%)
3	E	0.90	0/62	0.94	0/84
3	F	1.04	0/70	0.89	0/95
All	All	0.94	6/6778 (0.1%)	0.91	11/9210 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	6	GLU	CG-CD	-8.17	1.39	1.51
2	B	1	GLU	CD-OE2	6.76	1.33	1.25
2	H	6	GLU	CB-CG	6.50	1.64	1.52
1	A	23	CYS	CB-SG	6.38	1.93	1.82
1	A	86	GLU	CB-CG	5.94	1.63	1.52
2	H	32	TYR	CD2-CE2	5.68	1.47	1.39

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	66	ARG	NE-CZ-NH2	-14.21	113.19	120.30
1	A	66	ARG	NE-CZ-NH2	-11.35	114.62	120.30
1	L	66	ARG	NE-CZ-NH1	9.44	125.02	120.30
1	A	66	ARG	NE-CZ-NH1	9.18	124.89	120.30
1	L	9	LEU	CA-CB-CG	6.16	129.48	115.30
1	L	86	GLU	CA-CB-CG	5.72	125.99	113.40
1	A	149	LYS	CD-CE-NZ	5.41	124.14	111.70
1	L	11	LEU	CA-CB-CG	5.38	127.68	115.30
1	A	126	ASP	CB-CG-OD1	5.14	122.93	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	86	GLU	CB-CA-C	-5.11	100.19	110.40
2	H	179	LEU	CA-CB-CG	5.09	127.01	115.30

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	1659	0	1629	33	1
1	L	1659	0	1633	50	1
2	B	1591	0	1552	35	0
2	H	1587	0	1544	47	1
3	E	62	0	52	8	0
3	F	70	0	58	12	0
4	A	1	0	0	1	0
4	B	1	0	0	0	0
4	E	1	0	0	0	1
4	H	1	0	0	1	0
4	L	1	0	0	0	0
5	E	8	0	6	2	0
5	F	8	0	6	4	1
6	A	166	0	0	1	0
6	B	169	0	0	2	0
6	E	6	0	0	3	0
6	F	10	0	0	0	0
6	H	123	0	0	5	0
6	L	130	0	0	4	0
All	All	7253	0	6480	167	3

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 13.

All (167) 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:F:12:SER:C	5:F:101:OPE:N	1.77	1.37
3:E:12:SER:C	5:E:101:OPE:N	1.85	1.29
1:L:193:HIS:HD2	6:L:502:HOH:O	1.15	1.24
1:A:85:ALA:HA	1:A:110:ILE:HD11	1.26	1.13
3:F:12:SER:C	5:F:101:OPE:HN2	1.41	1.10
2:B:34:MET:HE2	2:B:100:PRO:HB3	1.34	1.06
1:L:155:ASP:OD2	1:L:193:HIS:ND1	1.88	1.03
2:H:106:GLN:HG2	6:H:501:HOH:O	1.60	1.01
2:B:34:MET:CE	2:B:100:PRO:HB3	1.90	1.01
3:E:12:SER:C	5:E:101:OPE:HN1	1.49	0.98
1:L:127:GLU:HG2	6:L:483:HOH:O	1.67	0.94
1:L:29:LEU:HD22	1:L:95:GLN:HG2	1.52	0.90
1:L:202:HIS:CD2	1:L:204:GLY:H	1.91	0.88
2:B:33:TRP:H	3:E:7:GLN:HE22	1.21	0.88
1:L:95:GLN:NE2	1:L:98:HIS:H	1.71	0.87
1:L:95:GLN:HE22	1:L:98:HIS:H	1.19	0.85
1:A:85:ALA:HA	1:A:110:ILE:CD1	2.09	0.83
1:L:193:HIS:CD2	6:L:502:HOH:O	2.02	0.83
1:L:202:HIS:HD2	1:L:204:GLY:H	1.25	0.83
1:A:66:ARG:NH2	1:A:87:ASP:OD2	2.14	0.81
1:A:142:ASN:OD1	2:H:1:GLU:HG2	1.80	0.81
1:A:142:ASN:OD1	2:H:1:GLU:CG	2.31	0.79
2:H:213:GLU:CB	2:H:214:PRO:HD3	2.13	0.79
2:H:189:SER:O	2:H:190:LEU:HB2	1.84	0.78
3:F:12:SER:C	5:F:101:OPE:HN1	1.82	0.77
2:B:53:LEU:H	2:B:56:ASN:HD22	1.33	0.76
1:A:95:GLN:HE22	1:A:98:HIS:H	1.32	0.76
2:H:35:ASN:OD1	2:H:50:GLN:HB3	1.87	0.75
1:L:13:VAL:HG21	1:L:83:VAL:HG21	1.69	0.75
2:H:185:VAL:HG12	6:H:458:HOH:O	1.87	0.75
1:L:95:GLN:HE21	1:L:97:SER:H	1.35	0.74
2:H:214:PRO:HA	6:H:412:HOH:O	1.88	0.74
1:L:95:GLN:HE21	1:L:97:SER:N	1.86	0.73
1:A:86:GLU:OE2	4:A:301:ZN:ZN	1.39	0.71
2:B:33:TRP:N	3:E:7:GLN:HE22	1.87	0.71
1:L:29:LEU:HD22	1:L:95:GLN:CG	2.21	0.70
1:A:100:HIS:HE1	6:E:205:HOH:O	1.74	0.70
2:H:213:GLU:HB2	2:H:214:PRO:HD3	1.73	0.70
2:H:53:LEU:H	2:H:56:ASN:HD22	1.38	0.70
3:E:4:ASP:HB2	6:E:206:HOH:O	1.91	0.69
3:F:3:ASN:O	3:F:4:ASP:HB2	1.92	0.69
1:A:202:HIS:CD2	1:A:204:GLY:H	2.10	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:53:ILE:HD12	1:L:78:LEU:HD13	1.74	0.69
2:H:50:GLN:NE2	2:H:52:ARG:HE	1.90	0.69
2:B:189:SER:HA	2:B:192:THR:HG22	1.73	0.69
3:F:5:THR:HG22	3:F:6:SER:N	2.09	0.68
1:L:162:ASN:HD22	1:L:162:ASN:H	1.41	0.68
1:A:202:HIS:HD2	1:A:204:GLY:H	1.41	0.67
2:B:206:THR:HG21	6:B:464:HOH:O	1.94	0.67
1:L:13:VAL:CG2	1:L:83:VAL:HG21	2.24	0.67
2:H:189:SER:O	2:H:190:LEU:CB	2.42	0.67
1:L:44:LYS:HG3	1:L:50:GLN:HE22	1.60	0.67
2:H:6:GLU:HG3	2:H:107:GLY:H	1.59	0.67
2:H:128:SER:OG	2:H:129:SER:N	2.27	0.66
2:H:1:GLU:OE1	4:H:301:ZN:ZN	1.46	0.65
1:L:187:LYS:O	1:L:191:GLU:HG2	1.97	0.64
1:L:95:GLN:NE2	1:L:97:SER:N	2.47	0.62
2:B:34:MET:HE1	2:B:100:PRO:HB3	1.78	0.62
3:F:12:SER:O	5:F:101:OPE:N	2.10	0.62
2:B:184:THR:HG23	2:H:3:GLN:OE1	2.01	0.61
2:B:1:GLU:HB3	2:B:3:GLN:NE2	2.15	0.61
1:L:169:GLU:HB3	6:L:471:HOH:O	2.01	0.61
2:H:50:GLN:HE21	2:H:52:ARG:HE	1.48	0.61
2:H:52:ARG:HB3	2:H:56:ASN:HD22	1.65	0.61
1:L:159:GLN:HB3	1:L:162:ASN:HD21	1.66	0.60
1:L:162:ASN:ND2	1:L:162:ASN:H	2.00	0.60
3:F:5:THR:HG22	3:F:6:SER:H	1.66	0.59
2:B:93:THR:HG23	2:B:111:THR:HA	1.84	0.59
2:H:33:TRP:CE2	2:H:52:ARG:HG2	2.37	0.59
2:H:57:ASN:HB2	6:H:468:HOH:O	2.02	0.59
1:L:146:ARG:CZ	1:L:167:VAL:HG21	2.34	0.58
1:A:53:ILE:HD12	1:A:78:LEU:HD13	1.86	0.58
1:A:79:LYS:HG3	6:A:455:HOH:O	2.04	0.57
1:L:202:HIS:HD2	1:L:204:GLY:N	2.00	0.57
2:B:136:THR:HG22	2:H:25:SER:HB2	1.87	0.57
1:A:33:ASN:ND2	1:A:35:LYS:H	2.02	0.57
1:A:84:GLU:OE1	1:L:66:ARG:HD3	2.04	0.56
2:H:6:GLU:HG3	2:H:107:GLY:N	2.21	0.56
1:A:142:ASN:OD1	2:H:1:GLU:OE1	2.25	0.55
1:A:128:GLN:HG2	1:A:133:THR:O	2.05	0.55
2:H:33:TRP:H	3:F:7:GLN:HE22	1.53	0.54
2:B:204:SER:OG	2:B:206:THR:HB	2.08	0.54
1:A:39:ASN:HB2	1:A:94:VAL:HG13	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:33:TRP:H	3:E:7:GLN:NE2	1.97	0.54
1:A:142:ASN:OD1	2:H:1:GLU:CD	2.47	0.54
1:L:14:THR:HG22	1:L:111:LYS:HB3	1.90	0.53
2:H:171:LEU:HD13	2:H:172:GLN:O	2.09	0.53
1:L:88:VAL:HG23	1:L:108:LEU:O	2.10	0.52
1:A:29:LEU:HD22	1:A:76:PHE:CE1	2.45	0.52
2:B:32:TYR:HB3	2:B:34:MET:HE3	1.92	0.51
1:A:33:ASN:HD22	1:A:33:ASN:C	2.13	0.51
1:A:155:ASP:O	1:A:156:ASN:HB2	2.08	0.51
1:L:13:VAL:HG21	1:L:83:VAL:CG2	2.39	0.51
2:B:189:SER:HA	2:B:192:THR:CG2	2.41	0.51
1:L:44:LYS:HG3	1:L:50:GLN:NE2	2.25	0.51
3:F:5:THR:O	3:F:6:SER:HB2	2.10	0.51
1:A:129:LEU:O	1:A:130:LYS:C	2.49	0.50
1:A:85:ALA:CA	1:A:110:ILE:HD11	2.18	0.50
1:L:167:VAL:HG22	1:L:179:LEU:HD12	1.94	0.50
2:H:199:VAL:O	2:H:207:LYS:HA	2.12	0.50
1:L:187:LYS:O	1:L:191:GLU:CG	2.60	0.49
2:B:1:GLU:CB	2:B:3:GLN:NE2	2.75	0.49
2:B:206:THR:CG2	6:B:464:HOH:O	2.57	0.49
1:L:145:PRO:O	1:L:202:HIS:HE1	1.95	0.49
1:L:66:ARG:NH2	1:L:87:ASP:OD2	2.36	0.49
1:L:29:LEU:HD12	1:L:76:PHE:CE2	2.47	0.49
2:H:33:TRP:N	3:F:7:GLN:HE22	2.11	0.48
2:B:1:GLU:HG3	1:L:141:ASN:OD1	2.13	0.48
1:L:84:GLU:HB3	1:L:86:GLU:OE1	2.13	0.48
2:B:184:THR:CG2	2:H:3:GLN:OE1	2.62	0.48
2:H:213:GLU:CB	2:H:214:PRO:CD	2.88	0.48
2:H:70:PHE:CZ	2:H:85:MET:HE2	2.49	0.48
2:H:30:SER:O	2:H:53:LEU:HD22	2.13	0.47
1:L:202:HIS:CD2	1:L:204:GLY:N	2.74	0.47
2:B:179:LEU:C	2:B:179:LEU:HD12	2.34	0.47
1:L:162:ASN:N	1:L:162:ASN:HD22	2.07	0.47
1:L:29:LEU:CD2	1:L:95:GLN:CG	2.91	0.47
2:H:171:LEU:HD13	2:H:171:LEU:C	2.35	0.47
1:L:88:VAL:HB	1:L:110:ILE:CD1	2.45	0.47
2:B:200:ASN:OD1	2:B:202:LYS:HG3	2.14	0.47
1:A:100:HIS:CE1	6:E:205:HOH:O	2.57	0.46
2:B:120:PRO:HD2	2:B:206:THR:HG21	1.97	0.46
2:H:27:PHE:HE2	2:H:34:MET:HE1	1.81	0.46
1:A:39:ASN:HD21	3:E:9:SER:HA	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:124:PRO:HD3	1:L:136:VAL:HG22	1.98	0.46
2:B:1:GLU:CB	2:B:3:GLN:HE22	2.29	0.45
2:H:70:PHE:N	2:H:70:PHE:CD1	2.83	0.45
1:A:203:GLN:HE21	1:A:203:GLN:HB3	1.61	0.45
3:F:5:THR:CG2	3:F:6:SER:N	2.79	0.45
2:H:213:GLU:HB3	2:H:214:PRO:HD3	1.97	0.45
2:B:85:MET:HE2	2:B:88:LEU:HD21	1.99	0.45
2:H:33:TRP:NE1	2:H:52:ARG:HG2	2.32	0.45
2:H:157:SER:HB3	6:H:507:HOH:O	2.17	0.45
1:A:196:TYR:O	1:A:212:SER:HA	2.17	0.44
1:A:33:ASN:ND2	1:A:33:ASN:C	2.71	0.44
1:A:66:ARG:HD3	1:L:84:GLU:OE1	2.17	0.44
1:L:195:VAL:HG22	1:L:214:ASN:HD22	1.82	0.44
2:H:127:PRO:O	2:H:128:SER:HB3	2.18	0.44
1:L:144:TYR:CG	1:L:145:PRO:HA	2.53	0.44
1:A:9:LEU:HA	1:A:9:LEU:HD12	1.87	0.44
1:L:95:GLN:HE22	1:L:98:HIS:N	2.01	0.44
2:B:120:PRO:HD2	2:B:206:THR:CG2	2.48	0.43
2:B:160:LEU:HD21	2:B:183:VAL:HG21	2.00	0.43
2:B:193:GLN:HE21	2:B:193:GLN:HB2	1.62	0.43
2:H:53:LEU:H	2:H:56:ASN:ND2	2.13	0.42
1:L:155:ASP:O	1:L:156:ASN:HB2	2.20	0.42
1:L:189:ASP:O	1:L:192:LYS:HB2	2.19	0.42
1:L:42:LEU:HD13	1:L:91:TYR:CZ	2.55	0.42
2:B:213:GLU:HB2	2:B:214:PRO:HD2	2.03	0.41
1:A:24:LYS:HE3	1:A:75:ASP:OD1	2.20	0.41
2:B:36:TRP:HD1	2:B:72:ILE:HD13	1.85	0.41
2:B:1:GLU:HB3	2:B:3:GLN:HE21	1.83	0.41
2:B:93:THR:HA	2:B:110:VAL:O	2.19	0.41
2:B:100:PRO:HD2	2:B:103:TYR:O	2.20	0.41
2:H:127:PRO:HA	2:H:138:ALA:O	2.19	0.41
2:H:66:VAL:O	2:H:67:LYS:C	2.59	0.41
2:H:70:PHE:N	2:H:70:PHE:HD1	2.19	0.41
1:A:149:LYS:HB3	1:A:201:THR:HB	2.03	0.41
2:B:38:ARG:HA	2:B:95:VAL:O	2.21	0.41
1:L:40:TRP:CE2	1:L:78:LEU:HB2	2.55	0.41
2:H:47:TRP:HZ2	2:H:50:GLN:HG2	1.86	0.41
1:A:33:ASN:HD22	1:A:35:LYS:H	1.69	0.40
1:L:192:LYS:HE2	1:L:192:LYS:HB3	1.80	0.40
2:H:33:TRP:CE2	3:F:12:SER:HA	2.57	0.40
2:H:12:VAL:HG11	2:H:88:LEU:HD13	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:33:TRP:CZ3	3:E:11:PRO:HD2	2.56	0.40
2:H:89:LYS:HD3	2:H:91:GLU:OE2	2.21	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:102:ZN:ZN	5:F:101:OPE:O1[2_354]	1.66	0.54
1:L:193:HIS:ND1	2:H:64:GLU:OE2[4_545]	2.00	0.20
1:A:1:ASP:OD1	1:A:189:ASP:OD2[4_455]	2.16	0.04

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	214/216 (99%)	205 (96%)	8 (4%)	1 (0%)	29 31
1	L	214/216 (99%)	203 (95%)	11 (5%)	0	100 100
2	B	207/216 (96%)	201 (97%)	5 (2%)	1 (0%)	29 31
2	H	207/216 (96%)	193 (93%)	10 (5%)	4 (2%)	8 5
3	E	7/10 (70%)	7 (100%)	0	0	100 100
3	F	8/10 (80%)	4 (50%)	2 (25%)	2 (25%)	0 0
All	All	857/884 (97%)	813 (95%)	36 (4%)	8 (1%)	17 16

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	F	4	ASP
3	F	6	SER
1	A	155	ASP
2	H	128	SER

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Mol	Chain	Res	Type
2	H	190	LEU
2	H	213	GLU
2	B	101	ILE
2	H	101	ILE

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	A	192/192 (100%)	183 (95%)	9 (5%)	26 33
1	L	192/192 (100%)	183 (95%)	9 (5%)	26 33
2	B	179/184 (97%)	162 (90%)	17 (10%)	8 8
2	H	179/184 (97%)	162 (90%)	17 (10%)	8 8
3	E	9/10 (90%)	8 (89%)	1 (11%)	6 5
3	F	10/10 (100%)	8 (80%)	2 (20%)	1 1
All	All	761/772 (99%)	706 (93%)	55 (7%)	14 15

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	29	LEU
1	A	33	ASN
1	A	95	GLN
1	A	109	GLU
1	A	131	SER
1	A	146	ARG
1	A	173	LYS
1	A	203	GLN
2	B	3	GLN
2	B	17	SER
2	B	21	SER
2	B	53	LEU
2	B	67	LYS

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Mol	Chain	Res	Type
2	B	90	THR
2	B	109	THR
2	B	136	THR
2	B	151	VAL
2	B	152	THR
2	B	162	SER
2	B	179	LEU
2	B	184	THR
2	B	192	THR
2	B	193	GLN
2	B	206	THR
2	B	207	LYS
1	L	13	VAL
1	L	58	LYS
1	L	86	GLU
1	L	101	THR
1	L	104	GLN
1	L	109	GLU
1	L	162	ASN
1	L	173	LYS
1	L	185	LEU
2	H	6	GLU
2	H	17	SER
2	H	19	ARG
2	H	78	LYS
2	H	98	CYS
2	H	102	ASP
2	H	106	GLN
2	H	114	SER
2	H	128	SER
2	H	151	VAL
2	H	152	THR
2	H	161	THR
2	H	179	LEU
2	H	180	SER
2	H	192	THR
2	H	194	THR
2	H	200	ASN
3	E	6	SER
3	F	3	ASN
3	F	12	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	39	ASN
1	A	50	GLN
1	A	95	GLN
1	A	100	HIS
1	A	202	HIS
1	A	203	GLN
2	B	3	GLN
2	B	56	ASN
2	B	57	ASN
2	B	193	GLN
1	L	27	GLN
1	L	50	GLN
1	L	95	GLN
1	L	162	ASN
1	L	202	HIS
1	L	214	ASN
2	H	50	GLN
2	H	56	ASN
2	H	61	HIS
2	H	86	ASN
2	H	165	HIS
2	H	193	GLN
2	H	200	ASN
3	E	7	GLN
3	F	7	GLN

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 (i)

Of 7 ligands modelled in this entry, 5 are monoatomic - leaving 2 for Mogul analysis.

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	OPE	F	101	-	7,7,7	0.61	0	9,9,9	1.01	0
5	OPE	E	101	4	7,7,7	0.63	0	9,9,9	1.72	2 (22%)

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	OPE	F	101	-	-	0/5/5/5	-
5	OPE	E	101	4	-	3/5/5/5	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	101	OPE	O4-P-O3	-3.68	96.16	106.47
5	E	101	OPE	O1-P-O4	2.36	113.01	106.73

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	101	OPE	O4-CA-CB-N
5	E	101	OPE	CA-O4-P-O1
5	E	101	OPE	CB-CA-O4-P

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	101	OPE	4	1
5	E	101	OPE	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	A	216/216 (100%)	-0.16	1 (0%) 91 90	17, 25, 39, 48	0
1	L	216/216 (100%)	-0.23	1 (0%) 91 90	18, 27, 40, 49	0
2	B	211/216 (97%)	-0.10	1 (0%) 91 90	17, 27, 40, 59	0
2	H	211/216 (97%)	0.06	4 (1%) 66 65	18, 29, 42, 52	0
3	E	9/10 (90%)	0.31	0 100 100	22, 25, 42, 47	0
3	F	10/10 (100%)	0.79	2 (20%) 1 1	22, 26, 52, 55	0
All	All	873/884 (98%)	-0.10	9 (1%) 82 81	17, 27, 40, 59	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	214	PRO	5.5
2	B	134	GLY	5.4
3	F	3	ASN	4.6
2	H	134	GLY	3.3
2	H	133	SER	2.9
3	F	4	ASP	2.9
1	L	156	ASN	2.7
1	A	216	GLY	2.6
2	H	129	SER	2.4

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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, 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	B-factors(Å^2)	Q<0.9
4	ZN	E	102	1/1	0.79	0.22	30,30,30,30	1
5	OPE	E	101	8/8	0.93	0.16	44,49,51,51	0
5	OPE	F	101	8/8	0.94	0.18	23,36,40,44	0
4	ZN	B	301	1/1	0.97	0.18	30,30,30,30	1
4	ZN	H	301	1/1	0.97	0.08	30,30,30,30	0
4	ZN	A	301	1/1	0.99	0.14	30,30,30,30	0
4	ZN	L	301	1/1	0.99	0.02	30,30,30,30	0

6.5 Other polymers

There are no such residues in this entry.