Full wwPDB X-ray Structure Validation Report (i)

Feb 26, 2014 – 03:15 PM GMT

PDB ID   :   3AJH
Title   :   Crystal structure of PcyA V225D-biliverdin XIII alpha complex
Authors   :   Wada, K.; Hagiwara, Y.; Fukuyama, K.
Deposited on :   2010-06-05
Resolution   :   2.25 Å(reported)

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

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1   Overall quality at a glance   ⓘ

The reported resolution of this entry is 2.25 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.
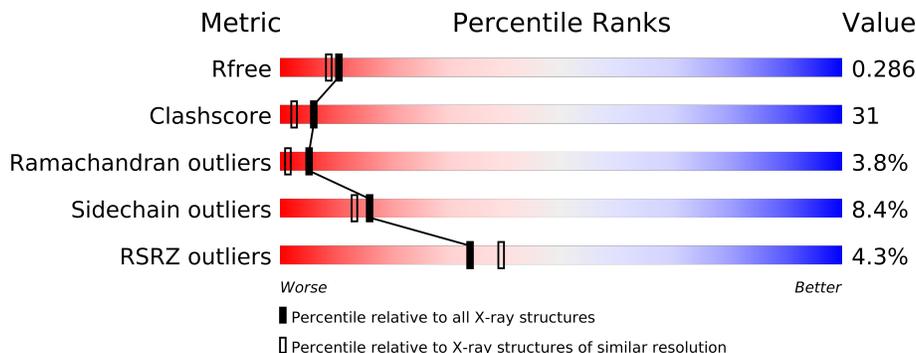
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1108 (2.28-2.24)
Clashscore	79885	1326 (2.28-2.24)
Ramachandran outliers	78287	1291 (2.28-2.24)
Sidechain outliers	78261	1291 (2.28-2.24)
RSRZ outliers	66119	1110 (2.28-2.24)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	248	
1	B	248	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	BL3	B	250	-	X

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 4064 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Phycocyanobilin:ferredoxinoxidoreductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	240	Total	C	N	O	S	0	0	0
			1918	1220	328	359	11			
1	B	241	Total	C	N	O	S	0	0	0
			1926	1226	329	360	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	225	ASP	VAL	ENGINEERED MUTATION	UNP Q55891
B	225	ASP	VAL	ENGINEERED MUTATION	UNP Q55891

- Molecule 2 is 3-[2-[(Z)-[3-(2-CARBOXYETHYL)-5-[(Z)-(3-ETHENYL-4-METHYL-5-OXO -PYRROL-2-YLIDENE)METHYL]-4-METHYL-PYRROL-2-YLIDENE]METHYL]-5-[(Z)- (3-ETHENYL-4-METHYL-5-OXO-PYRROL-2-YLIDENE)METHYL]-4-METHYL-1H-PY RROL-3-YL]PROPANOICACID (three-letter code: BL3) (formula: $C_{33}H_{34}N_4O_6$).
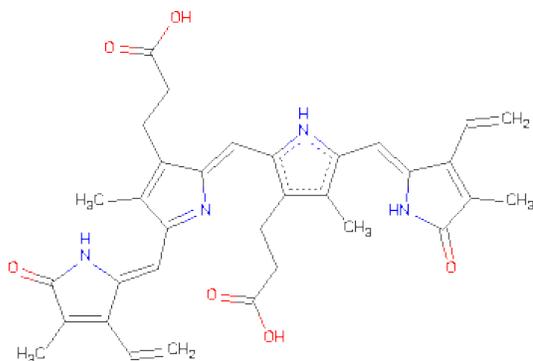
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 43	C 33	N 4	O 6	0	0
2	B	1	Total 43	C 33	N 4	O 6	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	63	Total 63	O 63	0	0
3	B	71	Total 71	O 71	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Phycocyanobilin:ferredoxinoxidoreductase

Chain A:
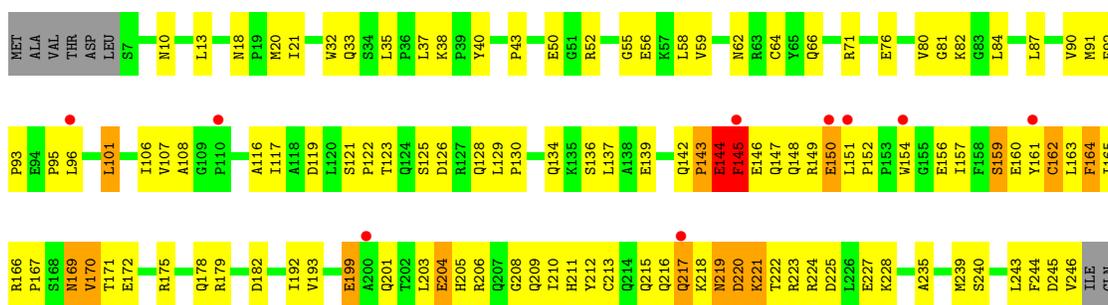
• Molecule 1: Phycocyanobilin:ferredoxinoxidoreductase

Chain B:
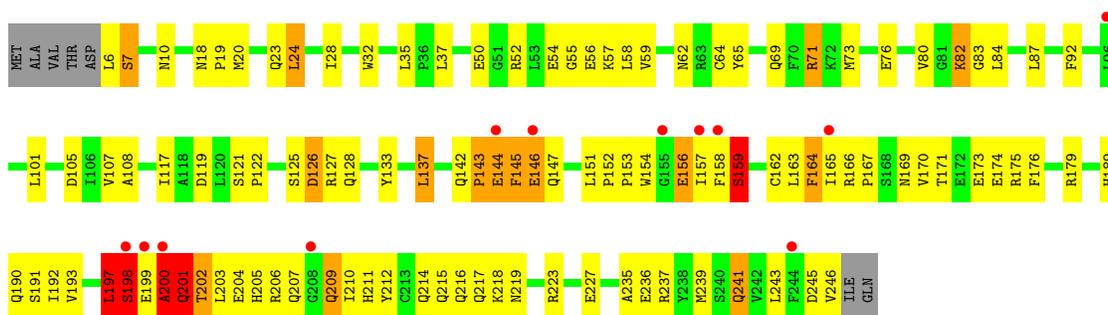
4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	74.61Å 74.61Å 84.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.98 – 2.25 27.98 – 2.25	Depositor EDS
% Data completeness (in resolution range)	97.9 (27.98-2.25) 97.8 (27.98-2.25)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	7.45 (at 2.24Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.251 , 0.289 0.251 , 0.286	Depositor DCC
R_{free} test set	1087 reflections (4.82%)	DCC
Wilson B-factor (Å^2)	42.5	Xtriage
Anisotropy	0.383	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 40.4	EDS
Estimated twinning fraction	0.487 for k,h,-l	Xtriage
L-test for twinning	$<|L|> = 0.49, <L^2> = 0.32$	Xtriage
Outliers	2 of 22968 reflections (0.009%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4064	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.25% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: BL3

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	0.46	0/1964	0.82	7/2664 (0.3%)
1	B	0.45	1/1972 (0.1%)	1.01	17/2675 (0.6%)
All	All	0.45	1/3936 (0.0%)	0.92	24/5339 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	201	GLN	N-CA	-6.17	1.34	1.46

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	199	GLU	CA-C-N	-14.15	86.08	117.20
1	B	201	GLN	N-CA-C	-14.13	72.84	111.00
1	B	200	ALA	CA-C-N	-12.63	89.42	117.20
1	B	198	SER	O-C-N	-10.31	106.20	122.70
1	A	145	PHE	N-CA-C	10.06	138.15	111.00
1	B	198	SER	CA-C-N	8.89	136.75	117.20
1	B	199	GLU	C-N-CA	8.53	143.02	121.70
1	B	200	ALA	C-N-CA	8.34	142.55	121.70
1	B	200	ALA	N-CA-CB	7.95	121.22	110.10
1	B	199	GLU	CA-C-O	7.81	136.49	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	144	GLU	C-N-CA	7.30	139.95	121.70
1	B	199	GLU	N-CA-CB	7.28	123.71	110.60
1	B	199	GLU	O-C-N	7.03	133.96	122.70
1	A	145	PHE	CA-C-N	-6.99	101.83	117.20
1	B	200	ALA	CA-C-O	6.66	134.08	120.10
1	A	145	PHE	C-N-CA	6.54	138.06	121.70
1	B	200	ALA	CB-CA-C	6.36	119.63	110.10
1	B	197	LEU	O-C-N	-5.94	113.19	122.70
1	B	198	SER	CB-CA-C	5.79	121.11	110.10
1	B	197	LEU	C-N-CA	5.64	135.81	121.70
1	B	198	SER	C-N-CA	5.62	135.75	121.70
1	A	145	PHE	CB-CG-CD1	5.22	124.45	120.80
1	A	145	PHE	O-C-N	5.12	130.90	122.70
1	A	175	ARG	C-N-CA	-5.07	109.02	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	200	ALA	Mainchain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1918	0	1885	106	0
1	B	1926	0	1896	125	0
2	A	43	0	32	14	0
2	B	43	0	32	4	0
3	A	63	0	0	13	0
3	B	71	0	0	13	0
All	All	4064	0	3845	241	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 31.

All (241) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:250:BL3:HMC	2:B:250:BL3:HBC	1.40	1.01
2:A:250:BL3:HMC	2:A:250:BL3:HBC	1.40	1.00
1:B:82:LYS:HG2	1:B:83:GLY:N	1.80	0.95
1:B:204:GLU:HB2	3:B:259:HOH:O	1.77	0.84
1:B:157:ILE:HG21	1:B:211:HIS:CD2	2.17	0.80
1:A:50:GLU:HG3	1:A:59:VAL:HG22	1.64	0.80
1:B:127:ARG:HE	1:B:157:ILE:HG22	1.47	0.80
1:B:200:ALA:HB1	1:B:203:LEU:H	1.46	0.79
1:A:220:ASP:O	1:A:224:ARG:HB3	1.82	0.79
1:B:200:ALA:HA	1:B:202:THR:N	1.96	0.78
1:A:151:LEU:HB3	3:A:273:HOH:O	1.84	0.78
1:A:150:GLU:O	1:A:150:GLU:HG2	1.85	0.77
1:B:197:LEU:O	1:B:201:GLN:HG3	1.85	0.76
1:B:209:GLN:O	1:B:212:TYR:HB3	1.86	0.76
1:B:203:LEU:HD11	3:B:278:HOH:O	1.84	0.75
1:A:143:PRO:HB3	3:A:292:HOH:O	1.87	0.75
1:B:142:GLN:CD	1:B:143:PRO:HD2	2.08	0.74
1:B:189:HIS:CD2	1:B:190:GLN:HE21	2.06	0.73
1:A:208:GLY:HA2	3:A:278:HOH:O	1.89	0.73
1:B:198:SER:OG	1:B:201:GLN:HG3	1.90	0.71
1:B:200:ALA:HA	1:B:202:THR:HB	1.72	0.71
1:B:237:ARG:O	1:B:241:GLN:HB2	1.91	0.70
1:A:217:GLN:NE2	1:A:239:MET:HB3	2.06	0.69
1:B:126:ASP:O	1:B:128:GLN:HG2	1.93	0.69
2:A:250:BL3:CMB	2:A:250:BL3:HBB	2.23	0.68
1:A:58:LEU:HD13	1:A:80:VAL:HG13	1.76	0.68
1:B:156:GLU:OE1	1:B:157:ILE:HG23	1.93	0.68
1:B:58:LEU:HD23	1:B:80:VAL:HG13	1.75	0.67
1:B:143:PRO:HD3	1:B:179:ARG:NH1	2.08	0.67
1:B:200:ALA:HA	1:B:202:THR:CB	2.25	0.67
1:A:223:ARG:O	1:A:227:GLU:HG3	1.96	0.66
1:B:84:LEU:HD11	1:B:107:VAL:HG13	1.77	0.66
1:A:221:LYS:HZ3	2:A:250:BL3:CBD	2.08	0.66
1:B:154:TRP:HA	1:B:215:GLN:NE2	2.11	0.66
1:B:23:GLN:NE2	3:B:274:HOH:O	2.28	0.65
1:A:169:ASN:C	1:A:171:THR:H	1.98	0.65
1:B:239:MET:CE	1:B:243:LEU:HD12	2.26	0.65
1:B:142:GLN:OE1	1:B:143:PRO:HD2	1.95	0.65
1:A:148:GLN:HG2	1:A:149:ARG:H	1.59	0.65
1:A:128:GLN:HA	1:A:128:GLN:HE21	1.62	0.65
1:A:122:PRO:HD3	1:A:159:SER:HB2	1.78	0.64
1:B:24:LEU:CD1	1:B:28:ILE:HD11	2.28	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:250:BL3:HBB	2:B:250:BL3:CMB	2.27	0.64
1:B:157:ILE:HG21	1:B:211:HIS:HD2	1.61	0.63
1:B:215:GLN:O	1:B:218:LYS:HB2	1.97	0.63
1:A:179:ARG:NH1	3:A:292:HOH:O	2.30	0.63
1:B:117:ILE:HG13	1:B:163:LEU:O	1.98	0.63
1:B:211:HIS:HA	1:B:214:GLN:OE1	1.98	0.62
1:B:206:ARG:HA	1:B:209:GLN:HB3	1.81	0.62
1:A:101:LEU:HB3	1:A:121:SER:HB2	1.81	0.62
1:B:52:ARG:HH21	1:B:55:GLY:C	2.03	0.62
1:A:56:GLU:HB3	1:A:81:GLY:HA2	1.82	0.61
1:B:202:THR:O	1:B:205:HIS:N	2.32	0.61
1:A:219:ASN:ND2	2:A:250:BL3:C1C	2.64	0.61
1:A:146:GLU:O	1:A:147:GLN:HB2	2.01	0.60
1:A:221:LYS:NZ	2:A:250:BL3:HBD	2.17	0.60
1:A:52:ARG:NH2	1:A:55:GLY:O	2.35	0.59
1:A:221:LYS:HZ3	2:A:250:BL3:HBD	1.68	0.58
1:A:125:SER:OG	1:A:204:GLU:HG3	2.03	0.58
1:B:197:LEU:HD23	1:B:201:GLN:HB3	1.86	0.58
1:A:159:SER:OG	1:A:160:GLU:N	2.33	0.58
1:B:133:TYR:O	1:B:137:LEU:HB2	2.03	0.58
1:B:202:THR:N	3:B:259:HOH:O	2.37	0.57
1:B:50:GLU:HG3	1:B:59:VAL:HG22	1.86	0.57
1:A:130:PRO:O	1:A:134:GLN:HG3	2.04	0.57
1:B:82:LYS:HE2	1:B:83:GLY:H	1.70	0.57
1:B:170:VAL:HG12	1:B:174:GLU:HG3	1.86	0.57
1:A:221:LYS:NZ	2:A:250:BL3:CBD	2.68	0.56
1:A:123:THR:HG23	1:A:205:HIS:ND1	2.21	0.56
1:B:205:HIS:O	1:B:206:ARG:HG3	2.05	0.56
1:A:166:ARG:NH1	3:A:299:HOH:O	2.36	0.56
1:B:87:LEU:HD23	1:B:87:LEU:C	2.26	0.56
1:B:200:ALA:CB	1:B:203:LEU:H	2.18	0.56
1:A:221:LYS:HZ3	2:A:250:BL3:HBDA	1.71	0.55
1:A:215:GLN:OE1	1:A:218:LYS:HD2	2.06	0.55
1:A:147:GLN:OE1	1:A:166:ARG:HD3	2.07	0.55
1:A:157:ILE:HD13	1:A:215:GLN:HB2	1.89	0.55
1:A:213:CYS:HB3	1:A:244:PHE:HB3	1.89	0.55
1:A:40:TYR:HB3	1:A:64:CYS:HB3	1.88	0.54
1:B:57:LYS:HG2	1:B:59:VAL:HG23	1.89	0.54
1:A:129:LEU:HB2	3:A:289:HOH:O	2.07	0.54
1:A:126:ASP:O	1:A:126:ASP:OD2	2.26	0.54
1:B:206:ARG:NH2	3:B:306:HOH:O	2.41	0.54
1:A:58:LEU:HD13	1:A:80:VAL:HA	1.90	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:219:ASN:OD1	1:A:221:LYS:HD2	2.08	0.54
1:B:71:ARG:HH21	1:B:92:PHE:HB3	1.72	0.54
1:A:219:ASN:C	1:A:221:LYS:H	2.11	0.54
1:A:192:ILE:HG13	1:A:193:VAL:HG13	1.90	0.53
1:B:119:ASP:OD2	1:B:162:CYS:HB2	2.08	0.53
1:A:170:VAL:O	1:A:170:VAL:HG12	2.08	0.53
1:B:206:ARG:CA	1:B:209:GLN:HB3	2.39	0.53
1:B:144:GLU:O	1:B:145:PHE:HB2	2.08	0.53
1:A:145:PHE:CD1	1:A:165:ILE:HD13	2.43	0.53
1:B:19:PRO:O	1:B:23:GLN:HG3	2.09	0.52
1:B:56:GLU:OE1	1:B:82:LYS:NZ	2.37	0.52
1:B:144:GLU:O	1:B:145:PHE:CB	2.56	0.52
1:B:151:LEU:HD12	1:B:151:LEU:H	1.73	0.52
1:A:143:PRO:CB	3:A:292:HOH:O	2.53	0.52
1:A:136:SER:O	1:A:139:GLU:HG2	2.09	0.52
1:A:128:GLN:HA	1:A:128:GLN:NE2	2.24	0.52
1:B:163:LEU:HD11	1:B:179:ARG:HG2	1.92	0.51
1:A:84:LEU:HD11	1:A:107:VAL:HG13	1.90	0.51
1:B:58:LEU:HD13	1:B:58:LEU:C	2.31	0.51
1:A:18:ASN:ND2	1:A:20:MET:H	2.09	0.51
1:A:169:ASN:C	1:A:171:THR:N	2.65	0.51
1:B:71:ARG:HD2	1:B:92:PHE:HB3	1.92	0.51
1:B:198:SER:OG	1:B:201:GLN:CG	2.59	0.50
1:A:235:ALA:O	1:A:239:MET:HG2	2.11	0.50
1:A:143:PRO:O	1:A:144:GLU:CB	2.59	0.50
1:A:206:ARG:O	1:A:210:ILE:HG13	2.11	0.50
2:A:250:BL3:HMBB	2:A:250:BL3:HBB	1.94	0.50
1:B:207:GLN:NE2	3:B:278:HOH:O	2.44	0.50
1:B:239:MET:HE2	1:B:243:LEU:HD12	1.93	0.50
1:B:197:LEU:O	1:B:198:SER:OG	2.24	0.50
1:A:143:PRO:CG	3:A:292:HOH:O	2.60	0.50
1:A:143:PRO:O	1:A:143:PRO:HG2	2.12	0.50
1:A:84:LEU:HD12	1:A:108:ALA:O	2.12	0.50
1:B:71:ARG:CD	3:B:257:HOH:O	2.60	0.49
1:B:142:GLN:HG3	1:B:143:PRO:N	2.26	0.49
1:A:119:ASP:OD2	1:A:162:CYS:HB2	2.12	0.49
1:A:90:VAL:HG11	1:A:92:PHE:CZ	2.46	0.49
2:A:250:BL3:HMC	2:A:250:BL3:CBC	2.27	0.49
1:B:157:ILE:O	1:B:157:ILE:HD12	2.13	0.49
1:B:71:ARG:HD3	3:B:257:HOH:O	2.12	0.49
2:B:250:BL3:HMC	2:B:250:BL3:CBC	2.26	0.49
1:B:18:ASN:ND2	1:B:20:MET:H	2.10	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:62:ASN:OD1	1:B:76:GLU:HG3	2.14	0.48
1:A:146:GLU:O	1:A:147:GLN:CB	2.61	0.48
1:B:24:LEU:HD13	1:B:28:ILE:CD1	2.44	0.48
1:A:117:ILE:HG13	1:A:163:LEU:O	2.14	0.48
1:B:167:PRO:HB3	1:B:173:GLU:HG3	1.96	0.48
1:A:87:LEU:HD23	1:A:87:LEU:C	2.33	0.48
1:B:82:LYS:HE2	3:B:282:HOH:O	2.13	0.48
1:B:101:LEU:HD13	1:B:212:TYR:CD2	2.49	0.48
1:B:145:PHE:C	1:B:147:GLN:H	2.15	0.48
1:B:200:ALA:HB2	1:B:202:THR:HB	1.96	0.47
1:A:147:GLN:HE22	1:A:166:ARG:HH21	1.62	0.47
1:B:159:SER:O	1:B:162:CYS:HB3	2.14	0.47
1:B:200:ALA:CA	1:B:202:THR:HB	2.43	0.47
1:A:154:TRP:HB2	1:A:218:LYS:HD3	1.95	0.47
1:B:200:ALA:HA	1:B:202:THR:CA	2.45	0.47
1:B:202:THR:HG22	1:B:206:ARG:HD2	1.97	0.47
1:B:154:TRP:HB2	1:B:215:GLN:HB3	1.96	0.47
1:A:216:GLN:HA	1:A:216:GLN:OE1	2.14	0.47
1:B:223:ARG:HH22	1:B:236:GLU:HA	1.80	0.47
1:A:240:SER:O	1:A:245:ASP:HA	2.14	0.47
1:A:149:ARG:HB2	1:A:164:PHE:CG	2.50	0.47
1:A:93:PRO:CD	1:A:101:LEU:HD22	2.44	0.47
1:A:62:ASN:ND2	1:A:76:GLU:HG3	2.29	0.46
1:B:101:LEU:HB2	1:B:121:SER:HB2	1.96	0.46
1:B:145:PHE:C	1:B:147:GLN:N	2.68	0.46
1:A:160:GLU:C	1:A:162:CYS:H	2.18	0.46
1:A:142:GLN:NE2	3:A:306:HOH:O	2.48	0.46
1:B:145:PHE:O	1:B:147:GLN:N	2.49	0.46
1:A:142:GLN:NE2	1:A:142:GLN:HA	2.30	0.46
1:B:192:ILE:HG13	1:B:193:VAL:HG13	1.98	0.46
1:A:211:HIS:HB3	3:A:278:HOH:O	2.16	0.45
1:B:169:ASN:HD21	1:B:171:THR:HB	1.81	0.45
1:B:58:LEU:CD2	1:B:80:VAL:HG13	2.44	0.45
1:A:178:GLN:HE21	1:A:182:ASP:CG	2.20	0.45
1:A:152:PRO:HB2	1:A:154:TRP:CE3	2.52	0.45
1:A:119:ASP:HB2	1:A:162:CYS:HB2	1.98	0.45
1:B:6:LEU:O	1:B:7:SER:O	2.35	0.45
1:B:202:THR:C	1:B:204:GLU:N	2.67	0.45
1:B:142:GLN:HG3	1:B:143:PRO:O	2.17	0.45
1:A:56:GLU:HB3	1:A:81:GLY:CA	2.47	0.45
1:B:105:ASP:HB3	3:B:316:HOH:O	2.16	0.45
1:A:219:ASN:O	1:A:221:LYS:N	2.49	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:219:ASN:ND2	2:A:250:BL3:NC	2.65	0.45
1:B:198:SER:HG	1:B:201:GLN:HG3	1.81	0.45
1:A:169:ASN:O	1:A:171:THR:N	2.50	0.45
1:B:20:MET:HE2	1:B:176:PHE:CD1	2.52	0.45
1:B:245:ASP:OD2	1:B:245:ASP:C	2.55	0.45
1:B:82:LYS:CG	1:B:83:GLY:N	2.66	0.45
1:B:151:LEU:HA	1:B:152:PRO:HD3	1.72	0.44
1:A:38:LYS:HB2	1:A:38:LYS:NZ	2.32	0.44
1:B:151:LEU:HD12	1:B:151:LEU:N	2.33	0.44
1:A:178:GLN:NE2	1:A:182:ASP:OD1	2.50	0.44
1:B:10:ASN:ND2	3:B:293:HOH:O	2.47	0.44
1:A:215:GLN:OE1	1:A:215:GLN:HA	2.17	0.44
1:B:156:GLU:H	1:B:156:GLU:CD	2.20	0.44
1:A:151:LEU:N	1:A:151:LEU:CD1	2.80	0.44
1:A:38:LYS:O	1:A:66:GLN:N	2.50	0.44
1:B:84:LEU:HD12	1:B:108:ALA:O	2.17	0.44
2:A:250:BL3:HMBA	2:A:250:BL3:HBB	2.00	0.43
1:A:213:CYS:CB	1:A:244:PHE:HB3	2.48	0.43
1:B:189:HIS:CD2	1:B:190:GLN:NE2	2.82	0.43
1:A:160:GLU:HG3	1:A:161:TYR:N	2.34	0.43
1:A:179:ARG:CZ	3:A:292:HOH:O	2.65	0.43
1:A:154:TRP:CB	1:A:218:LYS:HD3	2.48	0.43
1:A:13:LEU:HD21	1:A:59:VAL:CG1	2.49	0.43
1:A:239:MET:SD	1:A:243:LEU:HD12	2.58	0.43
1:B:6:LEU:N	1:B:65:TYR:HH	2.17	0.43
1:B:235:ALA:O	1:B:239:MET:HG2	2.18	0.43
1:A:106:ILE:HD13	1:A:116:ALA:HA	2.01	0.43
1:B:144:GLU:O	1:B:145:PHE:CG	2.72	0.43
1:B:64:CYS:HA	1:B:73:MET:O	2.19	0.43
1:B:69:GLN:HG2	1:B:191:SER:O	2.19	0.43
1:A:199:GLU:HG2	1:A:199:GLU:H	1.46	0.42
2:A:250:BL3:CMB	2:A:250:BL3:CBB	2.97	0.42
1:B:154:TRP:CE3	1:B:218:LYS:HG2	2.54	0.42
1:B:24:LEU:CD1	1:B:28:ILE:CD1	2.97	0.42
1:B:171:THR:O	1:B:175:ARG:HB2	2.19	0.42
1:A:216:GLN:C	1:A:218:LYS:N	2.73	0.42
1:B:152:PRO:HD3	1:B:164:PHE:CE1	2.54	0.42
1:B:6:LEU:N	3:B:302:HOH:O	2.53	0.42
1:B:52:ARG:NH2	1:B:56:GLU:HA	2.34	0.42
1:B:165:ILE:HG13	1:B:166:ARG:N	2.34	0.42
1:A:224:ARG:O	1:A:228:LYS:HG3	2.19	0.42
1:A:95:PRO:HD2	3:A:296:HOH:O	2.18	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:245:ASP:O	1:B:246:VAL:HG22	2.19	0.42
1:B:125:SER:HB3	3:B:312:HOH:O	2.20	0.42
1:B:209:GLN:HE21	1:B:209:GLN:HB2	1.59	0.42
1:B:212:TYR:O	1:B:216:GLN:HG2	2.19	0.42
1:B:50:GLU:HA	1:B:58:LEU:O	2.20	0.42
1:A:146:GLU:HB2	1:A:172:GLU:OE1	2.20	0.42
1:A:157:ILE:HB	1:A:212:TYR:HD1	1.85	0.42
1:A:62:ASN:HD21	1:A:76:GLU:HG3	1.82	0.42
1:B:121:SER:HA	1:B:122:PRO:HD3	1.77	0.42
1:B:217:GLN:C	1:B:219:ASN:N	2.72	0.42
2:B:250:BL3:HMBB	2:B:250:BL3:HBB	2.00	0.41
1:B:32:TRP:HB3	1:B:37:LEU:HD11	2.01	0.41
1:B:126:ASP:OD1	1:B:128:GLN:HB2	2.21	0.41
1:A:32:TRP:HB3	1:A:37:LEU:HD11	2.02	0.41
1:B:152:PRO:HA	1:B:153:PRO:HD3	1.85	0.41
1:A:21:ILE:CD1	1:A:106:ILE:HB	2.51	0.41
1:A:71:ARG:HD3	1:A:209:GLN:OE1	2.19	0.41
1:A:91:MET:O	1:A:101:LEU:HD13	2.20	0.41
1:B:200:ALA:CB	1:B:202:THR:HB	2.50	0.41
1:A:119:ASP:CG	1:A:162:CYS:HB2	2.41	0.41
1:B:24:LEU:HD13	1:B:28:ILE:HD11	2.00	0.41
1:A:151:LEU:HD12	1:A:151:LEU:N	2.35	0.41
1:A:147:GLN:HE22	1:A:166:ARG:NH2	2.18	0.41
1:B:193:VAL:O	1:B:193:VAL:HG23	2.20	0.41
1:A:224:ARG:CG	1:A:225:ASP:N	2.83	0.41
1:B:158:PHE:O	1:B:159:SER:HB3	2.20	0.41
1:B:209:GLN:HG2	1:B:210:ILE:HD12	2.03	0.40
1:A:222:THR:HG23	2:A:250:BL3:HMBB	2.02	0.40
1:B:58:LEU:CD2	1:B:80:VAL:HA	2.50	0.40
1:B:52:ARG:NH2	1:B:55:GLY:O	2.52	0.40
1:A:117:ILE:HG23	3:A:301:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	238/248 (96%)	218 (92%)	13 (6%)	7 (3%)	7	2
1	B	239/248 (96%)	210 (88%)	18 (8%)	11 (5%)	4	1
All	All	477/496 (96%)	428 (90%)	31 (6%)	18 (4%)	5	1

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	145	PHE
1	A	220	ASP
1	B	7	SER
1	B	144	GLU
1	B	145	PHE
1	A	170	VAL
1	B	198	SER
1	B	201	GLN
1	B	164	PHE
1	B	202	THR
1	A	219	ASN
1	B	146	GLU
1	A	96	LEU
1	A	144	GLU
1	B	54	GLU
1	B	159	SER
1	B	143	PRO
1	A	167	PRO

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	209/216 (97%)	187 (90%)	22 (10%)	10	7
1	B	210/216 (97%)	197 (94%)	13 (6%)	26	24
All	All	419/432 (97%)	384 (92%)	35 (8%)	16	13

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	33	GLN
1	A	35	LEU
1	A	43	PRO
1	A	82	LYS
1	A	101	LEU
1	A	137	LEU
1	A	143	PRO
1	A	144	GLU
1	A	150	GLU
1	A	156	GLU
1	A	159	SER
1	A	162	CYS
1	A	164	PHE
1	A	169	ASN
1	A	199	GLU
1	A	201	GLN
1	A	203	LEU
1	A	204	GLU
1	A	217	GLN
1	A	221	LYS
1	A	246	VAL
1	B	24	LEU
1	B	35	LEU
1	B	71	ARG
1	B	82	LYS
1	B	126	ASP
1	B	137	LEU
1	B	146	GLU
1	B	156	GLU
1	B	159	SER
1	B	197	LEU
1	B	209	GLN
1	B	227	GLU
1	B	241	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	33	GLN
1	A	62	ASN
1	A	124	GLN

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Mol	Chain	Res	Type
1	A	128	GLN
1	A	134	GLN
1	A	178	GLN
1	A	189	HIS
1	A	217	GLN
1	A	219	ASN
1	B	18	ASN
1	B	41	GLN
1	B	69	GLN
1	B	124	GLN
1	B	178	GLN
1	B	189	HIS
1	B	211	HIS
1	B	241	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

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
2	BL3	A	250	-	46,46,46	2.08	17 (36%)	65,67,67	1.50	11 (16%)
2	BL3	B	250	-	46,46,46	2.16	16 (34%)	65,67,67	1.53	12 (18%)

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
2	BL3	A	250	-	-	0/26/74/74	0/4/4/4
2	BL3	B	250	-	-	0/26/74/74	0/4/4/4

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	250	BL3	CHA-C4D	7.42	1.40	1.35
2	A	250	BL3	CHA-C4D	6.96	1.39	1.35
2	A	250	BL3	C4D-C3D	-3.81	1.38	1.45
2	A	250	BL3	C4A-NA	-3.65	1.33	1.36
2	B	250	BL3	C4D-C3D	-3.62	1.39	1.45
2	B	250	BL3	C1A-NA	-3.30	1.33	1.36
2	B	250	BL3	C2B-C1B	-3.27	1.38	1.45
2	B	250	BL3	C3C-C4C	-3.13	1.38	1.45
2	A	250	BL3	C1D-C2D	-2.94	1.39	1.45
2	B	250	BL3	C4B-C3B	-2.90	1.38	1.47
2	A	250	BL3	C3C-C4C	-2.84	1.39	1.45
2	B	250	BL3	C1C-C2C	-2.78	1.39	1.47
2	B	250	BL3	C4A-NA	-2.67	1.34	1.36
2	A	250	BL3	C4B-C3B	-2.66	1.39	1.47
2	B	250	BL3	C1D-C2D	-2.66	1.39	1.45
2	B	250	BL3	CHB-C1B	2.64	1.40	1.34
2	B	250	BL3	C4C-NC	-2.61	1.33	1.37
2	A	250	BL3	C4C-NC	-2.59	1.33	1.37
2	A	250	BL3	CAB-C2B	-2.56	1.39	1.48
2	B	250	BL3	C1B-NB	-2.52	1.33	1.37
2	A	250	BL3	C1C-C2C	-2.44	1.40	1.47
2	A	250	BL3	C1B-NB	-2.44	1.33	1.37
2	B	250	BL3	C4D-ND	-2.40	1.33	1.38
2	B	250	BL3	CAC-C3C	-2.39	1.39	1.48
2	B	250	BL3	CAB-C2B	-2.37	1.39	1.48
2	A	250	BL3	CAC-C3C	-2.35	1.39	1.48
2	A	250	BL3	C4B-NB	-2.31	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	250	BL3	C2B-C1B	-2.30	1.40	1.45
2	A	250	BL3	CHB-C1B	2.09	1.39	1.34
2	A	250	BL3	C4D-ND	-2.06	1.33	1.38
2	B	250	BL3	C4A-CHB	-2.04	1.38	1.46
2	A	250	BL3	C1A-CHA	-2.01	1.38	1.46
2	A	250	BL3	CBB-CAB	2.01	1.39	1.29

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	250	BL3	CHD-C1D-ND	4.68	133.89	124.99
2	B	250	BL3	CHD-C1D-ND	4.33	133.23	124.99
2	A	250	BL3	C2A-C1A-CHA	-3.50	115.80	125.72
2	B	250	BL3	C2A-C1A-CHA	-3.29	116.39	125.72
2	B	250	BL3	C1A-CHA-C4D	-3.22	123.63	129.92
2	A	250	BL3	CHA-C4D-C3D	-3.02	117.74	125.48
2	B	250	BL3	C4C-CHD-C1D	-2.94	120.82	128.13
2	A	250	BL3	C4C-CHD-C1D	-2.84	121.05	128.13
2	B	250	BL3	CHA-C4D-C3D	-2.83	118.24	125.48
2	B	250	BL3	CHB-C1B-C2B	-2.66	118.58	127.48
2	B	250	BL3	CHD-C4C-NC	2.66	131.96	126.19
2	A	250	BL3	CHD-C1D-C2D	-2.61	118.58	125.10
2	B	250	BL3	CHD-C4C-C3C	-2.56	118.92	127.48
2	A	250	BL3	CAD-C3D-C4D	2.55	129.58	124.85
2	B	250	BL3	CHD-C1D-C2D	-2.49	118.89	125.10
2	A	250	BL3	CHD-C4C-C3C	-2.48	119.19	127.48
2	B	250	BL3	C3A-C4A-CHB	-2.36	119.04	125.72
2	A	250	BL3	CHD-C4C-NC	2.30	131.19	126.19
2	A	250	BL3	C3A-C4A-CHB	-2.30	119.19	125.72
2	A	250	BL3	CHB-C1B-C2B	-2.29	119.84	127.48
2	A	250	BL3	CHA-C4D-ND	2.28	132.81	128.59
2	B	250	BL3	C4A-C3A-C2A	2.06	108.45	107.04
2	B	250	BL3	CHA-C4D-ND	2.05	132.38	128.59

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers (i)

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 (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	240/248 (96%)	0.28	9 (3%) 38	44	22, 49, 82, 103	2 (0%)
1	B	241/248 (97%)	0.35	12 (4%) 28	32	23, 50, 90, 103	1 (0%)
All	All	481/496 (96%)	0.32	21 (4%) 34	37	22, 50, 86, 103	3 (0%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	155	GLY	4.7
1	B	200	ALA	4.3
1	B	158	PHE	4.3
1	A	154	TRP	4.2
1	A	150	GLU	3.9
1	A	151	LEU	3.3
1	B	96	LEU	3.3
1	A	110	PRO	3.1
1	A	145	PHE	3.0
1	B	157	ILE	2.9
1	B	198	SER	2.6
1	A	161	TYR	2.5
1	B	144	GLU	2.5
1	B	244	PHE	2.5
1	B	208	GLY	2.3
1	B	146	GLU	2.3
1	B	165	ILE	2.1
1	A	96	LEU	2.1
1	B	199	GLU	2.1
1	A	217	GLN	2.1
1	A	200	ALA	2.1

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	BL3	B	250	43/43	0.33	3.01	54,83,98,109	0
2	BL3	A	250	43/43	0.30	1.81	66,92,110,114	0

6.5 Other polymers (i)

There are no such residues in this entry.