Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:26 AM GMT

PDB ID	:	2H63
Title	:	Crystal Structure of Human Biliverdin Reductase A (CASP Target)
Authors	:	Kavanagh, K.; Elkins, J.; Ugochukwu, E.; Guo, K.; Pilka, E.; Lukacik, P.; Smee, C.; Papagrigoriou, E.; Bunkoczi, G.; Sundstrom, M.; Arrowsmith, C.; Weigelt, J.; Edwards, A.; von Delft, F.; Oppermann, U.; Structural Genomics Consortium (SGC)
Deposited on	:	2006-05-30
Resolution	:	2.70 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

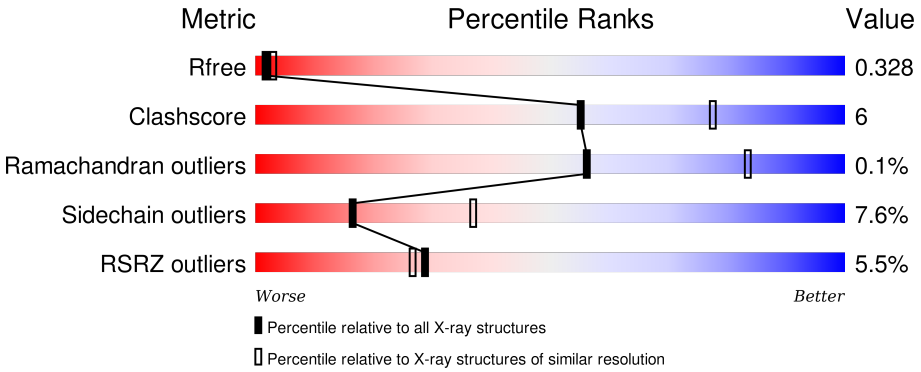
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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. 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	292	2% 83% 12%
1	B	292	4% 78% 16%
1	C	292	9% 79% 17%
1	D	292	5% 79% 17%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8668 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.

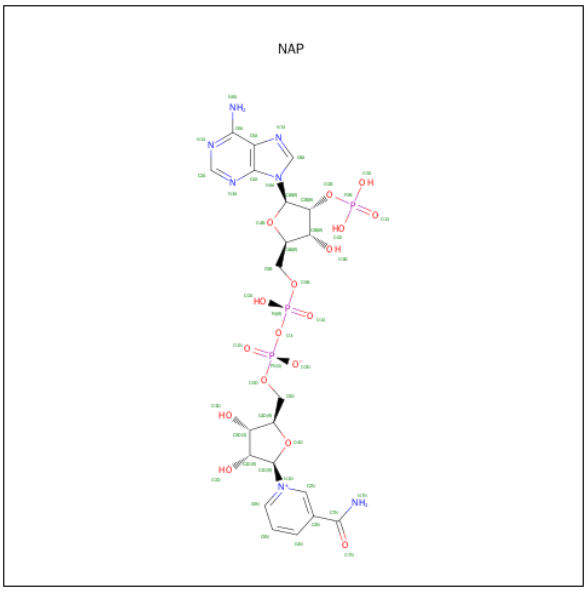
- Molecule 1 is a protein called Biliverdin reductase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	284	Total	C	N	O	S	0	0	0
			2140	1379	364	388	9			
1	B	279	Total	C	N	O	S	0	0	0
			2087	1342	359	378	8			
1	C	283	Total	C	N	O	S	0	0	0
			2097	1351	360	378	8			
1	D	285	Total	C	N	O	S	0	0	0
			2129	1375	360	385	9			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	5	SER	-	CLONING ARTIFACT	UNP P53004
A	6	MET	-	CLONING ARTIFACT	UNP P53004
B	5	SER	-	CLONING ARTIFACT	UNP P53004
B	6	MET	-	CLONING ARTIFACT	UNP P53004
C	5	SER	-	CLONING ARTIFACT	UNP P53004
C	6	MET	-	CLONING ARTIFACT	UNP P53004
D	5	SER	-	CLONING ARTIFACT	UNP P53004
D	6	MET	-	CLONING ARTIFACT	UNP P53004

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is water.

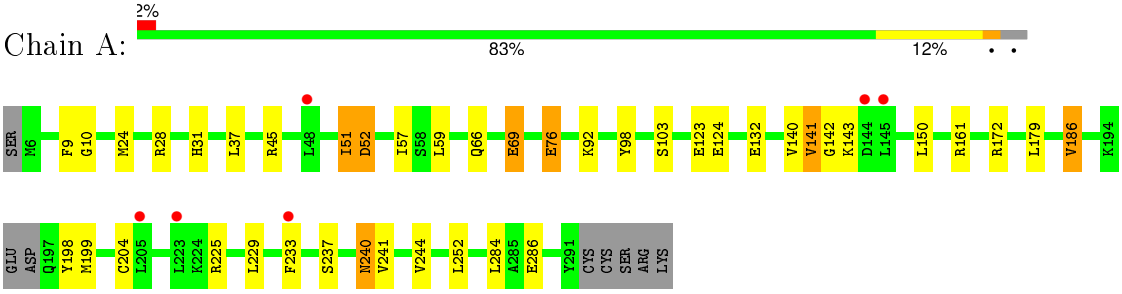
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	8	Total	O	0	0
			8	8		
3	B	4	Total	O	0	0
			4	4		
3	C	5	Total	O	0	0
			5	5		
3	D	6	Total	O	0	0
			6	6		

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 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.

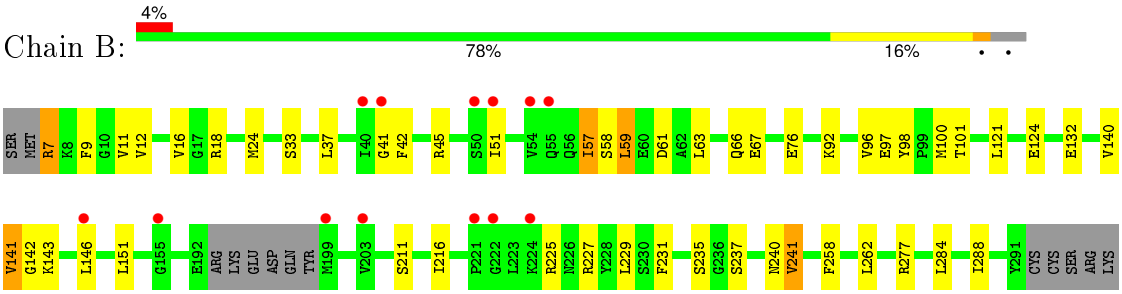
- Molecule 1: Biliverdin reductase A

Chain A:



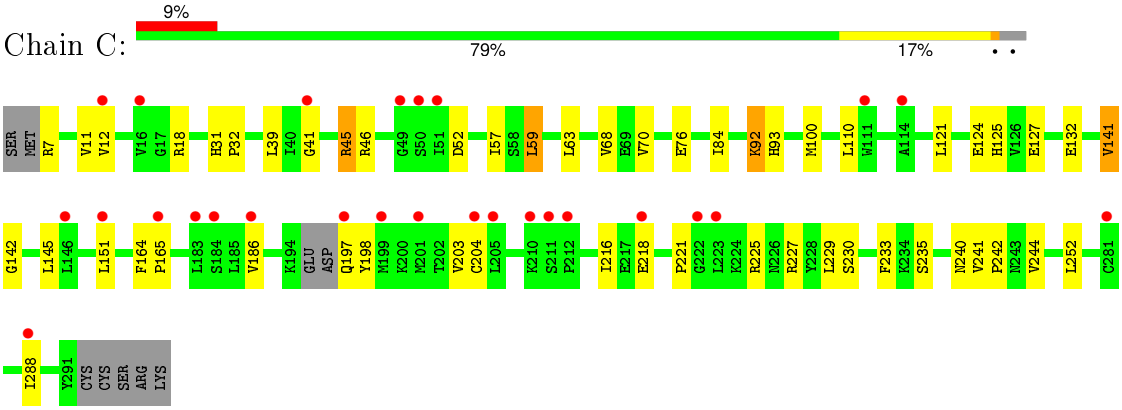
- Molecule 1: Biliverdin reductase A

Chain B:



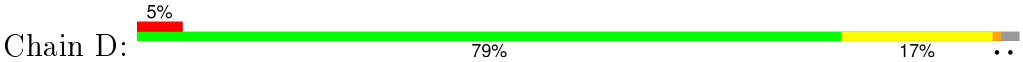
- Molecule 1: Biliverdin reductase A

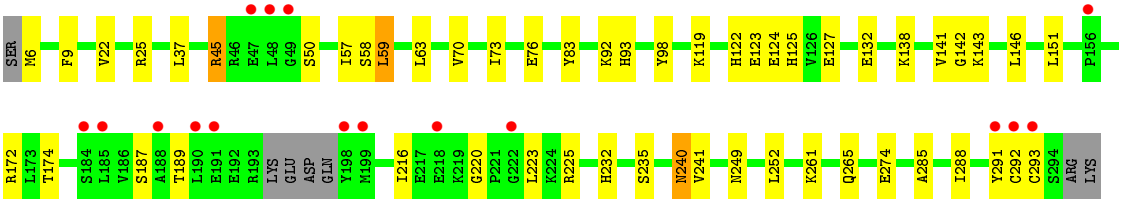
Chain C:



- Molecule 1: Biliverdin reductase A

Chain D:




SER M6 F9 V22 R25 L37 R45 R46 E47 L48 G49 S50 I57 S58 L59 L63 V70 I73 E76 Y83 K92 H93 Y98 K119 H122 E123 E124 H125 V126 E127 E132 K138 V141 G142 K143 L146 L151 P156
R172 L173 T174 S184 L185 V186 S187 A188 T189 L190 E191 E192 R193 LYS GLU ASP GLN Y198 M199 I216 E217 E218 K219 G220 P221 G222 L223 K224 R225 H232 S235 N240 V241 N249 L252 K261 Q265 E274 A285 I288 Y291 C292 C293 S294 ARG LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	90.79Å 92.75Å 147.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.70 41.30 – 2.70	Depositor EDS
% Data completeness (in resolution range)	96.4 (50.00-2.70) 96.4 (41.30-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.68 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.237 , 0.287 0.291 , 0.328	Depositor DCC
R_{free} test set	1399 reflections (4.33%)	DCC
Wilson B-factor (Å^2)	76.2	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 58.5	EDS
Estimated twinning fraction	0.006 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 33723 reflections	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	8668	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.83% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: NAP

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	0.73	2/2179 (0.1%)	0.71	0/2944
1	B	0.70	0/2125	0.74	2/2873 (0.1%)
1	C	0.67	0/2137	0.71	1/2895 (0.0%)
1	D	0.71	0/2169	0.73	1/2933 (0.0%)
All	All	0.71	2/8610 (0.0%)	0.73	4/11645 (0.0%)

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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	123	GLU	CB-CG	6.54	1.64	1.52
1	A	123	GLU	CG-CD	6.12	1.61	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	45	ARG	NE-CZ-NH2	5.75	123.18	120.30
1	C	227	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	B	277	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	B	227	ARG	NE-CZ-NH2	-5.03	117.79	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	240	ASN	Peptide

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	2140	0	2092	22	0
1	B	2087	0	2030	28	0
1	C	2097	0	2014	36	0
1	D	2129	0	2066	23	0
2	A	48	0	25	1	0
2	B	48	0	25	2	0
2	C	48	0	25	3	0
2	D	48	0	25	1	0
3	A	8	0	0	0	0
3	B	4	0	0	0	0
3	C	5	0	0	0	0
3	D	6	0	0	0	0
All	All	8668	0	8302	107	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 6.

All (107) 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:B:7:ARG:N	1:B:7:ARG:HD2	1.50	1.16
1:B:7:ARG:CD	1:B:7:ARG:N	2.19	1.06
1:C:242:PRO:O	1:C:244:VAL:HG23	1.80	0.80
1:D:132:GLU:HG3	1:D:241:VAL:HG11	1.67	0.77
1:C:229:LEU:HD23	1:C:230:SER:N	2.02	0.75
1:C:229:LEU:C	1:C:229:LEU:HD23	2.07	0.75
1:A:132:GLU:HG3	1:A:241:VAL:HG11	1.70	0.73
1:C:203:VAL:HG21	1:C:288:ILE:HD13	1.71	0.72
1:B:98:TYR:CE2	2:B:501:NAP:H5N	2.25	0.71
1:B:132:GLU:HG3	1:B:241:VAL:HG11	1.73	0.70
1:B:258:PHE:CE2	1:B:262:LEU:HD11	2.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:VAL:CG1	1:B:142:GLY:N	2.60	0.65
1:A:186:VAL:HG13	1:A:204:CYS:HB3	1.76	0.65
1:C:59:LEU:HD22	1:C:63:LEU:HD11	1.78	0.64
1:D:141:VAL:HG13	1:D:142:GLY:N	2.13	0.64
1:C:100:MET:HE1	1:C:121:LEU:HD21	1.81	0.63
1:D:70:VAL:HG22	1:D:93:HIS:HB2	1.80	0.62
1:C:244:VAL:O	1:C:244:VAL:HG12	1.99	0.61
1:B:42:PHE:CE1	1:B:51:ILE:HD12	2.35	0.61
1:D:123:GLU:OE1	1:D:125:HIS:NE2	2.35	0.60
1:C:132:GLU:HG3	1:C:241:VAL:HG11	1.83	0.60
1:A:24:MET:HE3	1:A:51:ILE:HG21	1.85	0.59
1:D:291:TYR:O	1:D:293:CYS:N	2.37	0.57
1:D:285:ALA:HA	1:D:288:ILE:HD12	1.87	0.57
1:C:59:LEU:HD22	1:C:63:LEU:CD1	2.33	0.57
1:B:24:MET:HE1	1:B:51:ILE:HD13	1.85	0.57
1:C:141:VAL:CG1	1:C:142:GLY:N	2.68	0.57
1:A:98:TYR:CE2	2:A:501:NAP:H5N	2.40	0.56
1:A:24:MET:CE	1:A:51:ILE:HG21	2.36	0.56
1:C:18:ARG:HD3	2:C:501:NAP:O2A	2.06	0.55
1:D:138:LYS:O	1:D:141:VAL:HG12	2.05	0.55
1:B:141:VAL:HG21	1:D:265:GLN:CG	2.35	0.55
1:A:150:LEU:HD21	1:A:172:ARG:HG3	1.89	0.55
1:C:145:LEU:HD12	1:C:233:PHE:CE1	2.42	0.55
1:C:84:ILE:CG2	1:C:110:LEU:HD13	2.37	0.55
1:C:164:PHE:CD1	1:C:165:PRO:HD2	2.42	0.55
1:C:141:VAL:HG13	1:C:142:GLY:N	2.22	0.54
1:C:84:ILE:HG21	1:C:110:LEU:HD13	1.90	0.54
1:C:229:LEU:CD2	1:C:229:LEU:C	2.76	0.54
1:C:12:VAL:HG23	1:C:41:GLY:O	2.08	0.54
1:D:151:LEU:HD13	1:D:216:ILE:HB	1.90	0.54
1:A:229:LEU:C	1:A:229:LEU:HD23	2.30	0.52
1:B:100:MET:HG3	1:B:101:THR:HG23	1.92	0.52
1:C:59:LEU:CD2	1:C:63:LEU:HD11	2.41	0.51
1:C:46:ARG:NE	2:C:501:NAP:O1X	2.43	0.50
1:C:11:VAL:O	1:C:39:LEU:HD12	2.13	0.49
1:A:51:ILE:HG22	1:A:52:ASP:N	2.26	0.49
1:B:229:LEU:HD21	1:B:231:PHE:CE2	2.48	0.49
1:B:12:VAL:HG23	1:B:41:GLY:O	2.12	0.49
1:B:57:ILE:HD12	1:B:58:SER:H	1.78	0.49
1:C:70:VAL:HG22	1:C:93:HIS:HB2	1.94	0.49
1:C:198:TYR:OH	1:C:218:GLU:OE2	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:7:ARG:N	1:C:7:ARG:CD	2.76	0.49
1:B:59:LEU:HD22	1:B:63:LEU:CD1	2.43	0.48
1:A:244:VAL:HG22	1:C:32:PRO:N	2.28	0.48
1:A:9:PHE:HB2	1:A:37:LEU:HD23	1.96	0.48
1:D:220:GLY:N	1:D:223:LEU:HD12	2.30	0.47
1:D:291:TYR:C	1:D:293:CYS:H	2.17	0.47
1:C:197:GLN:O	1:C:221:PRO:HD3	2.15	0.47
1:A:198:TYR:CD2	1:A:199:MET:N	2.83	0.47
1:B:151:LEU:HD13	1:B:216:ILE:HB	1.96	0.47
1:D:249:ASN:HB3	1:D:252:LEU:HB3	1.97	0.46
1:C:31:HIS:CG	1:C:252:LEU:HD21	2.51	0.46
1:B:141:VAL:HG12	1:B:142:GLY:N	2.29	0.46
1:D:141:VAL:CG1	1:D:142:GLY:N	2.79	0.46
1:B:11:VAL:CG2	1:B:37:LEU:HD22	2.46	0.46
1:A:103:SER:HA	1:A:286:GLU:OE2	2.16	0.45
1:B:9:PHE:HB2	1:B:37:LEU:HD23	1.97	0.45
1:C:186:VAL:HG13	1:C:204:CYS:HB3	1.99	0.45
1:B:141:VAL:HG13	1:B:142:GLY:N	2.32	0.45
1:C:68:VAL:O	1:C:92:LYS:NZ	2.40	0.45
1:C:151:LEU:HD13	1:C:216:ILE:CG2	2.47	0.44
1:A:240:ASN:HD22	1:A:240:ASN:N	2.14	0.44
1:D:98:TYR:CE2	2:D:501:NAP:H5N	2.52	0.44
1:C:45:ARG:NE	2:C:501:NAP:O3X	2.50	0.44
1:A:31:HIS:CG	1:A:252:LEU:HD21	2.53	0.44
1:C:125:HIS:ND1	1:C:127:GLU:OE2	2.51	0.44
1:B:57:ILE:HD12	1:B:58:SER:N	2.33	0.44
1:D:127:GLU:OE2	1:D:174:THR:HG21	2.18	0.44
1:D:261:LYS:NZ	1:D:274:GLU:OE1	2.51	0.43
1:A:143:LYS:HB3	1:A:233:PHE:CD1	2.53	0.43
1:D:22:VAL:HG13	1:D:25:ARG:NH2	2.33	0.43
1:A:140:VAL:HG21	1:A:179:LEU:HD22	1.99	0.43
1:A:186:VAL:HG13	1:A:204:CYS:CB	2.48	0.43
1:A:252:LEU:HD12	1:A:252:LEU:HA	1.75	0.43
1:B:241:VAL:O	1:B:241:VAL:HG12	2.18	0.43
1:D:93:HIS:CE1	1:D:119:LYS:HD3	2.53	0.43
1:C:186:VAL:HG13	1:C:204:CYS:CB	2.49	0.43
1:B:100:MET:CE	1:B:121:LEU:HD21	2.48	0.43
1:B:96:VAL:HG22	1:B:97:GLU:O	2.19	0.43
1:C:203:VAL:CG2	1:C:288:ILE:HD13	2.43	0.42
1:B:57:ILE:HD11	1:B:61:ASP:CB	2.49	0.42
1:B:229:LEU:C	1:B:229:LEU:HD23	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:ARG:HB2	2:B:501:NAP:O1N	2.20	0.42
1:D:240:ASN:N	1:D:240:ASN:ND2	2.67	0.42
1:C:203:VAL:HG12	1:C:204:CYS:N	2.35	0.42
1:D:122:HIS:ND1	1:D:261:LYS:NZ	2.58	0.42
1:D:73:ILE:HD12	1:D:83:TYR:HB3	2.01	0.42
1:A:284:LEU:HD23	1:A:284:LEU:HA	1.89	0.42
1:A:141:VAL:CG1	1:A:142:GLY:N	2.83	0.42
1:A:10:GLY:H	1:A:69:GLU:HG3	1.84	0.42
1:D:59:LEU:HD22	1:D:63:LEU:HD11	2.02	0.41
1:C:127:GLU:OE1	1:C:127:GLU:N	2.47	0.41
1:D:9:PHE:HB2	1:D:37:LEU:HD23	2.03	0.41
1:B:16:VAL:O	1:B:16:VAL:HG12	2.21	0.41
1:B:284:LEU:O	1:B:288:ILE:HG13	2.21	0.40
1:A:76:GLU:HG2	1:A:161:ARG:CZ	2.51	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	280/292 (96%)	264 (94%)	16 (6%)	0	100	100
1	B	275/292 (94%)	264 (96%)	11 (4%)	0	100	100
1	C	279/292 (96%)	268 (96%)	11 (4%)	0	100	100
1	D	281/292 (96%)	268 (95%)	12 (4%)	1 (0%)	39	69
All	All	1115/1168 (96%)	1064 (95%)	50 (4%)	1 (0%)	56	83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	292	CYS

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	216/255 (85%)	200 (93%)	16 (7%)	17 39
1	B	209/255 (82%)	190 (91%)	19 (9%)	12 26
1	C	206/255 (81%)	195 (95%)	11 (5%)	28 57
1	D	212/255 (83%)	194 (92%)	18 (8%)	13 30
All	All	843/1020 (83%)	779 (92%)	64 (8%)	16 37

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ARG
1	A	45	ARG
1	A	51	ILE
1	A	52	ASP
1	A	57	ILE
1	A	59	LEU
1	A	66	GLN
1	A	69	GLU
1	A	76	GLU
1	A	92	LYS
1	A	124	GLU
1	A	141	VAL
1	A	186	VAL
1	A	225	ARG
1	A	237	SER
1	A	240	ASN
1	B	7	ARG
1	B	33	SER
1	B	45	ARG
1	B	57	ILE
1	B	59	LEU
1	B	66	GLN
1	B	67	GLU
1	B	76	GLU

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Mol	Chain	Res	Type
1	B	92	LYS
1	B	124	GLU
1	B	140	VAL
1	B	141	VAL
1	B	143	LYS
1	B	146	LEU
1	B	211	SER
1	B	225	ARG
1	B	235	SER
1	B	237	SER
1	B	241	VAL
1	C	45	ARG
1	C	52	ASP
1	C	57	ILE
1	C	59	LEU
1	C	76	GLU
1	C	92	LYS
1	C	124	GLU
1	C	141	VAL
1	C	225	ARG
1	C	235	SER
1	C	240	ASN
1	D	6	MET
1	D	45	ARG
1	D	50	SER
1	D	57	ILE
1	D	58	SER
1	D	59	LEU
1	D	76	GLU
1	D	92	LYS
1	D	124	GLU
1	D	143	LYS
1	D	146	LEU
1	D	172	ARG
1	D	187	SER
1	D	189	THR
1	D	225	ARG
1	D	232	HIS
1	D	235	SER
1	D	240	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	240	ASN
1	B	55	GLN
1	C	255	GLN
1	D	240	ASN

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

4 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	NAP	A	501	-	42,52,52	1.17	4 (9%)	54,80,80	2.14	13 (24%)
2	NAP	B	501	-	42,52,52	1.30	4 (9%)	54,80,80	1.86	9 (16%)
2	NAP	C	501	-	42,52,52	1.27	4 (9%)	54,80,80	2.02	10 (18%)
2	NAP	D	501	-	42,52,52	1.37	5 (11%)	54,80,80	2.05	11 (20%)

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	NAP	A	501	-	-	0/27/67/67	0/5/5/5
2	NAP	B	501	-	-	0/27/67/67	0/5/5/5
2	NAP	C	501	-	-	0/27/67/67	0/5/5/5
2	NAP	D	501	-	-	0/27/67/67	0/5/5/5

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	NAP	P2B-O3X	-2.40	1.46	1.54
2	B	501	NAP	C5A-N7A	-2.19	1.32	1.39
2	A	501	NAP	PA-O2A	-2.13	1.45	1.54
2	D	501	NAP	P2B-O3X	-2.03	1.47	1.54
2	C	501	NAP	O5D-C5D	-2.01	1.36	1.44
2	C	501	NAP	C5B-C4B	2.07	1.58	1.51
2	D	501	NAP	C6N-N1N	2.18	1.41	1.35
2	A	501	NAP	P2B-O2X	2.31	1.63	1.54
2	D	501	NAP	P2B-O2X	2.60	1.64	1.54
2	D	501	NAP	C3N-C7N	2.84	1.55	1.50
2	B	501	NAP	O4D-C1D	2.96	1.44	1.41
2	A	501	NAP	P2B-O1X	2.97	1.60	1.51
2	A	501	NAP	O4B-C1B	3.47	1.45	1.41
2	C	501	NAP	C3N-C7N	3.51	1.56	1.50
2	C	501	NAP	P2B-O1X	3.82	1.63	1.51
2	B	501	NAP	P2B-O1X	4.09	1.64	1.51
2	D	501	NAP	P2B-O1X	4.88	1.67	1.51

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	501	NAP	N3A-C2A-N1A	-9.35	121.73	128.89
2	C	501	NAP	N3A-C2A-N1A	-8.79	122.16	128.89
2	B	501	NAP	N3A-C2A-N1A	-7.45	123.19	128.89
2	A	501	NAP	N3A-C2A-N1A	-6.83	123.66	128.89
2	A	501	NAP	O4B-C1B-N9A	-5.95	95.65	108.10
2	D	501	NAP	O4B-C1B-N9A	-5.47	96.65	108.10
2	A	501	NAP	O4D-C1D-N1N	-5.08	102.55	108.13
2	C	501	NAP	PN-O3-PA	-4.95	118.83	132.73
2	A	501	NAP	C4B-O4B-C1B	-4.65	104.60	109.72
2	A	501	NAP	O2B-P2B-O1X	-4.26	96.46	107.11
2	C	501	NAP	C4D-O4D-C1D	-4.19	105.12	109.72
2	B	501	NAP	C4D-O4D-C1D	-4.15	105.16	109.72
2	D	501	NAP	PN-O3-PA	-3.93	121.69	132.73
2	C	501	NAP	O4D-C1D-N1N	-3.93	103.81	108.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	NAP	PN-O3-PA	-3.85	121.91	132.73
2	A	501	NAP	P2B-O2B-C2B	-3.63	112.86	121.56
2	B	501	NAP	PN-O3-PA	-3.42	123.12	132.73
2	A	501	NAP	O3-PN-O5D	-3.06	94.81	102.94
2	B	501	NAP	C3N-C7N-N7N	-2.93	114.61	117.82
2	D	501	NAP	C4B-O4B-C1B	-2.89	106.54	109.72
2	D	501	NAP	O2B-P2B-O1X	-2.79	100.14	107.11
2	C	501	NAP	C4B-O4B-C1B	-2.68	106.78	109.72
2	A	501	NAP	C3N-C2N-N1N	-2.64	117.31	120.36
2	A	501	NAP	C4D-O4D-C1D	-2.60	106.87	109.72
2	B	501	NAP	C4B-O4B-C1B	-2.45	107.03	109.72
2	D	501	NAP	C5D-C4D-C3D	-2.35	105.88	115.21
2	C	501	NAP	O2D-C2D-C3D	-2.29	104.37	111.83
2	B	501	NAP	C3N-C2N-N1N	-2.28	117.73	120.36
2	D	501	NAP	C4D-O4D-C1D	-2.15	107.35	109.72
2	C	501	NAP	O2X-P2B-O1X	-2.12	103.75	110.58
2	A	501	NAP	C5D-C4D-C3D	-2.02	107.18	115.21
2	A	501	NAP	C3N-C7N-N7N	-2.02	115.61	117.82
2	D	501	NAP	O4D-C1D-N1N	-2.01	105.92	108.13
2	D	501	NAP	C3N-C7N-N7N	-2.01	115.62	117.82
2	D	501	NAP	O2A-PA-O1A	2.00	123.37	112.53
2	C	501	NAP	C5N-C4N-C3N	2.35	123.29	120.33
2	C	501	NAP	O2A-PA-O3	2.36	115.79	105.09
2	B	501	NAP	O7N-C7N-N7N	2.62	126.29	122.59
2	C	501	NAP	O3X-P2B-O1X	2.72	119.33	110.58
2	D	501	NAP	O3-PA-O5B	2.78	110.32	102.94
2	B	501	NAP	O3X-P2B-O1X	3.26	121.09	110.58
2	A	501	NAP	C2N-C3N-C4N	3.61	122.31	118.29
2	B	501	NAP	C2N-C3N-C4N	4.13	122.89	118.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	NAP	1	0
2	B	501	NAP	2	0
2	C	501	NAP	3	0
2	D	501	NAP	1	0

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, 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	284/292 (97%)	0.42	6 (2%) 67 68	48, 71, 74, 79	0
1	B	279/292 (95%)	0.47	13 (4%) 35 34	48, 71, 74, 79	0
1	C	283/292 (96%)	0.69	27 (9%) 10 8	48, 71, 74, 79	0
1	D	285/292 (97%)	0.56	16 (5%) 28 26	49, 71, 74, 80	0
All	All	1131/1168 (96%)	0.54	62 (5%) 29 27	48, 71, 74, 80	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	222	GLY	4.1
1	C	223	LEU	3.8
1	C	197	GLN	3.8
1	C	50	SER	3.8
1	B	41	GLY	3.6
1	B	222	GLY	3.6
1	A	48	LEU	3.5
1	D	49	GLY	3.5
1	D	47	GLU	3.5
1	D	199	MET	3.4
1	C	212	PRO	3.2
1	C	288	ILE	3.2
1	C	218	GLU	3.2
1	A	205	LEU	3.1
1	C	201	MET	3.1
1	B	55	GLN	3.0
1	D	190	LEU	3.0
1	D	292	CYS	2.9
1	C	222	GLY	2.8
1	C	184	SER	2.8
1	A	223	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	199	MET	2.8
1	D	48	LEU	2.8
1	C	205	LEU	2.8
1	B	199	MET	2.7
1	B	224	LYS	2.6
1	C	210	LYS	2.6
1	D	218	GLU	2.6
1	C	49	GLY	2.6
1	D	185	LEU	2.6
1	C	114	ALA	2.5
1	C	51	ILE	2.5
1	D	156	PRO	2.5
1	C	204	CYS	2.4
1	D	188	ALA	2.4
1	B	203	VAL	2.4
1	D	291	TYR	2.4
1	B	40	ILE	2.4
1	A	233	PHE	2.3
1	C	165	PRO	2.3
1	B	155	GLY	2.3
1	C	151	LEU	2.3
1	C	16	VAL	2.3
1	C	186	VAL	2.3
1	D	191	GLU	2.2
1	A	145	LEU	2.2
1	C	12	VAL	2.2
1	C	211	SER	2.2
1	C	41	GLY	2.1
1	D	293	CYS	2.1
1	B	54	VAL	2.1
1	B	51	ILE	2.1
1	B	221	PRO	2.1
1	C	281	CYS	2.1
1	B	50	SER	2.1
1	C	146	LEU	2.1
1	A	144	ASP	2.1
1	B	146	LEU	2.0
1	C	183	LEU	2.0
1	C	111	TRP	2.0
1	D	184	SER	2.0
1	D	198	TYR	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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, 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	LLDF	B-factors(Å^2)	Q<0.9
2	NAP	D	501	48/48	0.93	0.17	-1.12	58,69,76,81	0
2	NAP	A	501	48/48	0.94	0.15	-1.13	48,56,63,65	0
2	NAP	C	501	48/48	0.92	0.17	-1.31	57,65,82,84	0
2	NAP	B	501	48/48	0.94	0.15	-1.62	61,69,81,82	0

6.5 Other polymers (i)

There are no such residues in this entry.