Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:31 AM GMT

PDB ID	:	2DDS
Title	:	Crystal structure of sphingomyelinase from Bacillus cereus with cobalt ion
Authors	:	Ago, H.; Oda, M.; Takahashi, M.; Tsuge, H.; Ochi, S.; Katunuma, N.; Miyano, M.; Sakurai, J.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2006-02-02
Resolution	:	1.80 Å(reported)

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

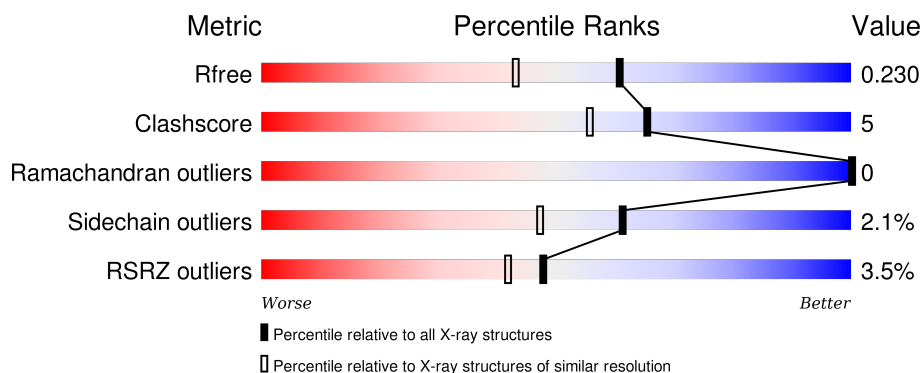|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 1.80 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	Percentile Ranks	Value
Rfree		0.230
Clashscore		5
Ramachandran outliers		0
Sidechain outliers		2.1%
RSRZ outliers		3.5%

Worse   *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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 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	306	3% 86% 11% ••
1	B	306	4% 82% 12% 6%
1	C	306	3% 88% 9% ••
1	D	306	4% 84% 10% 5%

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
2	CO	A	1127	-	-	-	X
2	CO	B	1125	-	-	-	X
2	CO	C	1126	-	-	-	X
2	CO	D	1128	-	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10448 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 Sphingomyelin phosphodiesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	299	Total 2364	C 1489	N 395	O 472	S 8	0	0	0
1	B	288	Total 2289	C 1447	N 382	O 454	S 6	0	0	0
1	C	298	Total 2356	C 1485	N 393	O 470	S 8	0	0	0
1	D	291	Total 2311	C 1458	N 386	O 461	S 6	0	0	0

- Molecule 2 is COBALT (II) ION (three-letter code: CO) (formula: Co).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	3	Total 3	Co 3	0	0
2	A	3	Total 3	Co 3	0	0
2	D	3	Total 3	Co 3	0	0
2	C	3	Total 3	Co 3	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	304	Total 304	O 304	0	0
3	B	261	Total 261	O 261	0	0
3	C	281	Total 281	O 281	0	0
3	D	270	Total 270	O 270	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.
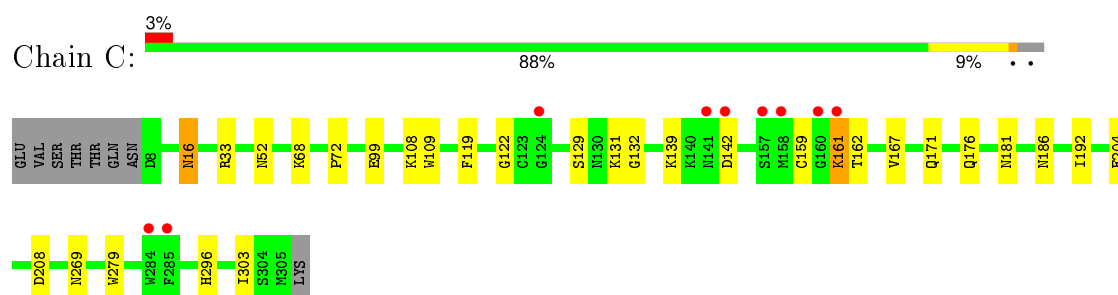
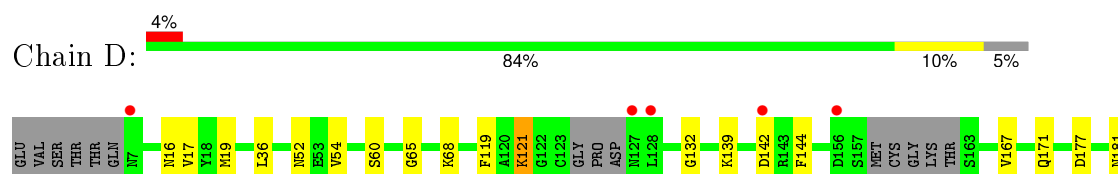- Molecule 1: Sphingomyelin phosphodiesterase
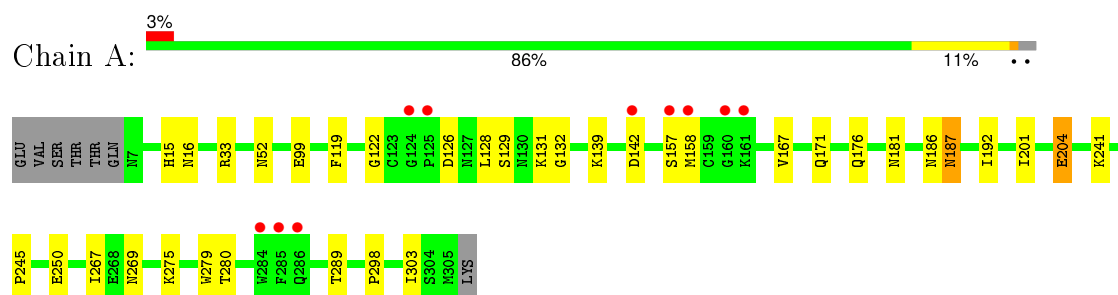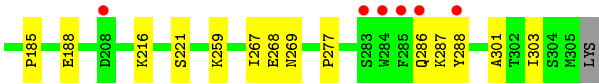

- Molecule 1: Sphingomyelin phosphodiesterase
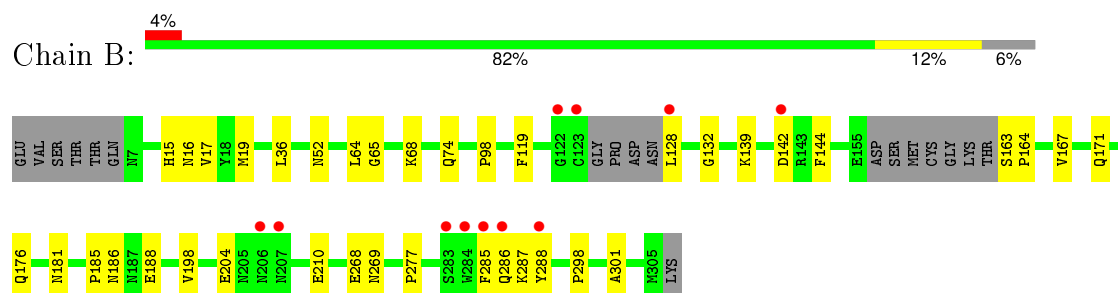
- Molecule 1: Sphingomyelin phosphodiesterase

- Molecule 1: Sphingomyelin phosphodiesterase

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	65.09Å　　72.67Å　　78.06Å 112.00°　　90.05°　　116.58°	Depositor
Resolution (Å)	19.67　–　1.80 35.80　–　1.77	Depositor EDS
% Data completeness (in resolution range)	91.6 (19.67-1.80) 77.8 (35.80-1.77)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.81 (at 1.77Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.202　，　0.232 0.199　，　0.230	Depositor DCC
R_{free} test set	9874 reflections (10.02%)	DCC
Wilson B-factor (Å^2)	16.9	Xtriage
Anisotropy	0.331	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 24.8	EDS
Estimated twinning fraction	0.486 for h,-h-k,-l	Xtriage
L-test for twinning [2]	$< |L| > = 0.50, < L^2 > = 0.34$	Xtriage
Outliers	0 of 103230 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10448	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 75.13 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.3416e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[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 (i)

5.1 Standard geometry (i)

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

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	0.30	0/2421	0.59	0/3295
1	B	0.30	0/2343	0.57	0/3187
1	C	0.30	0/2413	0.59	0/3284
1	D	0.29	0/2365	0.57	0/3217
All	All	0.30	0/9542	0.58	0/12983

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	2364	0	2264	25	0
1	B	2289	0	2198	21	0
1	C	2356	0	2258	24	0
1	D	2311	0	2213	22	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
2	D	3	0	0	0	0
3	A	304	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	261	0	0	0	0
3	C	281	0	0	1	0
3	D	270	0	0	1	0
All	All	10448	0	8933	92	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 5.

All (92) 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:D:139:LYS:HE2	1:D:142:ASP:HA	1.46	0.97
1:B:139:LYS:HE2	1:B:142:ASP:HA	1.52	0.91
1:C:139:LYS:HE2	1:C:142:ASP:HA	1.67	0.77
1:C:161:LYS:HD2	1:C:161:LYS:H	1.52	0.74
1:A:280:THR:HG22	1:A:289:THR:HG22	1.71	0.72
1:D:65:GLY:HA2	1:D:68:LYS:HE2	1.72	0.71
1:A:126:ASP:HB2	1:A:128:LEU:HD11	1.73	0.69
1:B:65:GLY:HA2	1:B:68:LYS:HE2	1.74	0.69
1:C:16:ASN:HA	1:C:52:ASN:HB2	1.76	0.67
1:A:16:ASN:HA	1:A:52:ASN:HB2	1.77	0.66
1:B:16:ASN:HA	1:B:52:ASN:HB2	1.78	0.65
1:D:17:VAL:HG23	1:D:19:MET:HG3	1.80	0.64
1:D:139:LYS:HD3	1:D:144:PHE:CE2	2.33	0.64
1:B:139:LYS:HD3	1:B:144:PHE:CE2	2.34	0.62
1:C:16:ASN:OD1	1:C:296:HIS:CD2	2.54	0.61
1:B:17:VAL:HG23	1:B:19:MET:HG3	1.83	0.61
1:A:122:GLY:HA2	1:A:167:VAL:HG11	1.83	0.60
1:A:139:LYS:HE2	1:A:142:ASP:HA	1.82	0.60
1:C:122:GLY:HA2	1:C:167:VAL:HG11	1.85	0.59
1:A:167:VAL:O	1:A:171:GLN:HG3	2.03	0.57
1:B:139:LYS:HE2	1:B:142:ASP:CA	2.31	0.57
1:D:16:ASN:HA	1:D:52:ASN:HB2	1.87	0.56
1:A:128:LEU:N	1:A:128:LEU:HD12	2.21	0.55
1:C:139:LYS:HE2	1:C:142:ASP:CA	2.36	0.55
1:C:167:VAL:O	1:C:171:GLN:HG3	2.06	0.54
1:C:204:GLU:H	1:C:204:GLU:CD	2.09	0.54
1:D:139:LYS:HE2	1:D:142:ASP:CA	2.28	0.53
1:B:167:VAL:O	1:B:171:GLN:HG3	2.08	0.53
1:C:161:LYS:HB3	1:C:161:LYS:HZ2	1.74	0.52
1:C:303:ILE:HD12	1:C:303:ILE:N	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:SER:HB3	1:B:164:PRO:HD3	1.91	0.52
1:A:204:GLU:CD	1:A:204:GLU:H	2.12	0.52
1:D:185:PRO:HB2	1:D:188:GLU:HG3	1.92	0.52
1:C:119:PHE:CD1	1:C:132:GLY:HA2	2.45	0.52
1:A:119:PHE:CD1	1:A:132:GLY:HA2	2.45	0.51
1:D:119:PHE:CD1	1:D:132:GLY:HA2	2.46	0.51
1:C:161:LYS:HD2	1:C:161:LYS:N	2.23	0.51
1:A:280:THR:CG2	1:A:289:THR:HG22	2.38	0.51
1:C:131:LYS:HE2	3:C:1191:HOH:O	2.12	0.49
1:A:131:LYS:HE2	3:A:1175:HOH:O	2.11	0.49
1:B:285:PHE:O	1:B:286:GLN:HB2	2.13	0.49
1:B:119:PHE:CD1	1:B:132:GLY:HA2	2.48	0.49
1:B:185:PRO:HB2	1:B:188:GLU:HG3	1.95	0.48
1:D:221:SER:HA	1:D:259:LYS:HE3	1.95	0.48
1:B:268:GLU:O	1:B:301:ALA:HA	2.14	0.47
1:A:241:LYS:O	1:A:245:PRO:HG3	2.14	0.47
1:C:161:LYS:NZ	1:C:161:LYS:HB3	2.28	0.47
1:B:204:GLU:H	1:B:204:GLU:CD	2.18	0.47
1:A:33:ARG:HD3	1:A:279:TRP:CZ2	2.50	0.46
1:C:33:ARG:HD3	1:C:279:TRP:CZ2	2.50	0.46
1:B:36:LEU:HD22	1:B:277:PRO:HG2	1.98	0.46
1:C:108:LYS:HG3	1:C:109:TRP:CD1	2.51	0.46
1:D:303:ILE:N	1:D:303:ILE:HD12	2.30	0.46
1:C:119:PHE:CE1	1:C:132:GLY:HA2	2.51	0.46
1:D:268:GLU:O	1:D:301:ALA:HA	2.16	0.46
1:C:161:LYS:CD	1:C:161:LYS:H	2.24	0.46
1:D:286:GLN:HG2	1:D:287:LYS:N	2.29	0.46
1:D:119:PHE:CE1	1:D:132:GLY:HA2	2.52	0.45
1:D:167:VAL:O	1:D:171:GLN:HG3	2.15	0.45
1:D:54:VAL:HB	1:D:60:SER:HB2	1.97	0.45
1:D:267:ILE:HG13	1:D:303:ILE:HG13	1.98	0.45
1:A:267:ILE:HG13	1:A:303:ILE:HG13	1.99	0.45
1:C:99:GLU:O	1:C:129:SER:HA	2.16	0.44
1:C:159:CYS:HB3	1:C:162:THR:O	2.18	0.44
1:A:119:PHE:CE1	1:A:132:GLY:HA2	2.53	0.43
1:A:99:GLU:O	1:A:129:SER:HA	2.17	0.43
1:C:122:GLY:HA2	1:C:167:VAL:CG1	2.48	0.43
1:A:303:ILE:N	1:A:303:ILE:HD12	2.34	0.42
1:B:98:PRO:HD2	1:B:128:LEU:HA	2.00	0.42
1:B:64:LEU:HB3	1:B:74:GLN:HE22	1.84	0.42
1:D:216:LYS:HB3	1:D:216:LYS:HE2	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:GLN:HG2	1:B:287:LYS:N	2.34	0.42
1:D:121:LYS:N	1:D:121:LYS:HD2	2.35	0.42
1:D:65:GLY:HA2	1:D:68:LYS:CE	2.45	0.42
1:A:122:GLY:HA2	1:A:167:VAL:CG1	2.49	0.42
1:B:15:HIS:CG	1:B:298:PRO:HB3	2.55	0.42
1:A:201:ILE:HD12	1:A:250:GLU:HA	2.00	0.42
1:B:198:VAL:HG13	1:B:210:GLU:HG2	2.02	0.42
1:D:177:ASP:HB3	3:D:1317:HOH:O	2.20	0.41
1:A:187:ASN:C	1:A:187:ASN:HD22	2.23	0.41
1:A:187:ASN:C	1:A:187:ASN:ND2	2.75	0.41
1:D:36:LEU:HD22	1:D:277:PRO:CG	2.51	0.41
1:B:119:PHE:CE1	1:B:132:GLY:HA2	2.56	0.41
1:C:68:LYS:HD2	1:C:72:PRO:HA	2.03	0.41
1:A:157:SER:HB2	1:A:158:MET:SD	2.61	0.41
1:A:192:ILE:HD12	1:A:192:ILE:N	2.35	0.41
1:C:16:ASN:OD1	1:C:296:HIS:CG	2.73	0.40
1:B:65:GLY:HA2	1:B:68:LYS:CE	2.49	0.40
1:A:15:HIS:CG	1:A:298:PRO:HB3	2.57	0.40
1:C:192:ILE:N	1:C:192:ILE:HD12	2.36	0.40
1:D:68:LYS:HB2	1:D:68:LYS:HE2	1.86	0.40
1:A:275:LYS:HD3	1:A:275:LYS:HA	1.92	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	297/306 (97%)	286 (96%)	11 (4%)	0	100	100
1	B	282/306 (92%)	271 (96%)	11 (4%)	0	100	100
1	C	296/306 (97%)	286 (97%)	10 (3%)	0	100	100
1	D	285/306 (93%)	277 (97%)	8 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1160/1224 (95%)	1120 (97%)	40 (3%)	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	263/270 (97%)	257 (98%)	6 (2%)	58 42
1	B	254/270 (94%)	249 (98%)	5 (2%)	63 49
1	C	262/270 (97%)	255 (97%)	7 (3%)	52 36
1	D	257/270 (95%)	253 (98%)	4 (2%)	70 59
All	All	1036/1080 (96%)	1014 (98%)	22 (2%)	61 47

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	176	GLN
1	A	181	ASN
1	A	186	ASN
1	A	187	ASN
1	A	204	GLU
1	A	269	ASN
1	B	176	GLN
1	B	181	ASN
1	B	186	ASN
1	B	269	ASN
1	B	288	TYR
1	C	16	ASN
1	C	161	LYS
1	C	176	GLN
1	C	181	ASN
1	C	186	ASN
1	C	208	ASP

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Mol	Chain	Res	Type
1	C	269	ASN
1	D	121	LYS
1	D	181	ASN
1	D	269	ASN
1	D	288	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	74	GLN
1	A	92	ASN
1	A	176	GLN
1	A	181	ASN
1	A	183	ASN
1	A	186	ASN
1	A	187	ASN
1	A	207	ASN
1	A	219	ASN
1	A	243	ASN
1	B	23	ASN
1	B	74	GLN
1	B	92	ASN
1	B	141	ASN
1	B	176	GLN
1	B	181	ASN
1	B	183	ASN
1	B	186	ASN
1	B	243	ASN
1	B	278	GLN
1	C	23	ASN
1	C	74	GLN
1	C	92	ASN
1	C	176	GLN
1	C	181	ASN
1	C	183	ASN
1	C	186	ASN
1	C	207	ASN
1	C	243	ASN
1	C	273	GLN
1	C	278	GLN
1	D	23	ASN

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Mol	Chain	Res	Type
1	D	74	GLN
1	D	92	ASN
1	D	176	GLN
1	D	181	ASN
1	D	183	ASN
1	D	243	ASN
1	D	261	HIS
1	D	278	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	299/306 (97%)	-0.22	10 (3%)	50	44	8, 15, 34, 51	0
1	B	288/306 (94%)	-0.23	11 (3%)	44	38	8, 16, 34, 42	0
1	C	298/306 (97%)	-0.25	9 (3%)	54	48	8, 15, 34, 52	0
1	D	291/306 (95%)	-0.17	11 (3%)	44	38	9, 16, 37, 49	0
All	All	1176/1224 (96%)	-0.22	41 (3%)	48	42	8, 15, 35, 52	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	160	GLY	5.1
1	C	285	PHE	4.5
1	A	285	PHE	4.3
1	D	288	TYR	4.1
1	D	128	LEU	3.9
1	C	124	GLY	3.9
1	D	284	TRP	3.9
1	C	142	ASP	3.8
1	D	142	ASP	3.7
1	B	288	TYR	3.4
1	C	161	LYS	3.3
1	B	142	ASP	3.2
1	A	284	TRP	3.2
1	A	142	ASP	3.1
1	A	158	MET	3.1
1	D	156	ASP	3.1
1	B	284	TRP	2.9
1	B	286	GLN	2.9
1	B	206	ASN	2.8
1	D	7	ASN	2.8
1	A	124	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	128	LEU	2.7
1	B	207	ASN	2.6
1	A	286	GLN	2.6
1	D	208	ASP	2.6
1	B	123	CYS	2.5
1	D	127	ASN	2.5
1	A	161	LYS	2.5
1	B	283	SER	2.5
1	D	285	PHE	2.4
1	D	283	SER	2.4
1	C	284	TRP	2.4
1	C	158	MET	2.4
1	B	122	GLY	2.3
1	A	160	GLY	2.3
1	B	285	PHE	2.2
1	A	157	SER	2.0
1	D	286	GLN	2.0
1	C	141	ASN	2.0
1	A	125	PRO	2.0
1	C	157	SER	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, 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	LLDF	B-factors(Å^2)	Q<0.9
2	CO	D	1128	1/1	0.86	0.20	14.19	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	CO	B	1125	1/1	0.80	0.20	11.91	107,107,107,107	0
2	CO	A	1127	1/1	0.97	0.14	5.97	63,63,63,63	0
2	CO	C	1126	1/1	0.97	0.18	4.19	63,63,63,63	0
2	CO	B	1122	1/1	0.99	0.06	-1.24	20,20,20,20	0
2	CO	A	1121	1/1	0.98	0.05	-2.22	19,19,19,19	0
2	CO	D	1124	1/1	0.99	0.03	-3.84	21,21,21,21	0
2	CO	C	1123	1/1	0.99	0.03	-4.11	19,19,19,19	0
2	CO	D	1120	1/1	0.99	0.03	-	20,20,20,20	0
2	CO	C	1119	1/1	0.99	0.04	-	21,21,21,21	0
2	CO	B	1118	1/1	0.98	0.04	-	19,19,19,19	0
2	CO	A	1117	1/1	0.97	0.04	-	21,21,21,21	0

6.5 Other polymers (i)

There are no such residues in this entry.