



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 2, 2021 – 08:43 AM EDT

PDB ID : 2DD9
Title : A mutant of GFP-like protein from *Chiridius poppei*
Authors : Suto, K.; Masuda, H.; Takenaka, Y.; Mizuno, H.
Deposited on : 2006-01-24
Resolution : 2.30 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 : 2.23.2
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) : 2.23.2

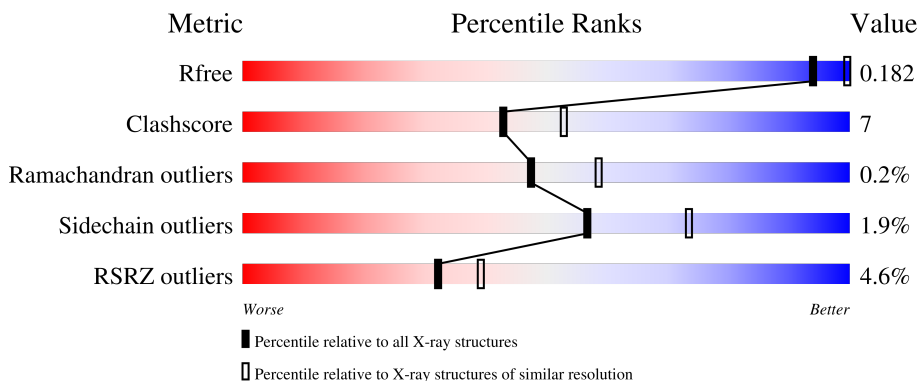
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	216	 3% 81% 18%
1	B	216	 3% 88% 11%
1	C	216	 6% 85% 12% ..
1	D	216	 6% 82% 15% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7436 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.

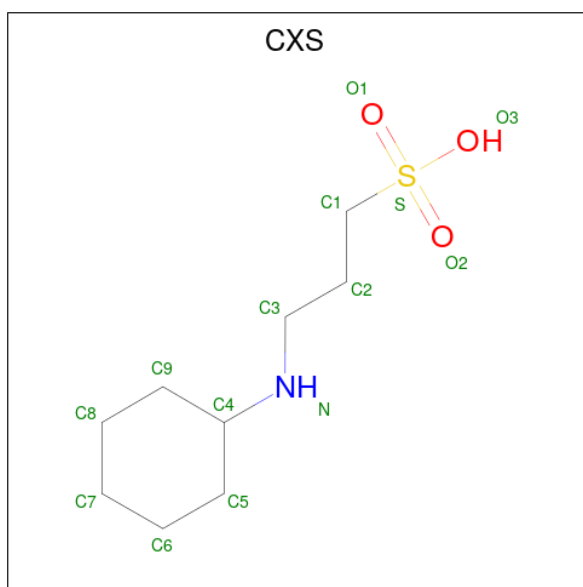
- Molecule 1 is a protein called green fluorescent protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	215	1721	1099	288	325	9	0	0	0
1	B	215	1721	1099	288	325	9	0	0	0
1	C	214	1713	1095	287	322	9	0	0	0
1	D	215	1721	1099	288	325	9	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	52	THR	HIS	engineered mutation	UNP Q2MHN7
A	56	CR2	GLY	chromophore	UNP Q2MHN7
A	56	CR2	TYR	chromophore	UNP Q2MHN7
A	56	CR2	GLY	chromophore	UNP Q2MHN7
B	52	THR	HIS	engineered mutation	UNP Q2MHN7
B	56	CR2	GLY	chromophore	UNP Q2MHN7
B	56	CR2	TYR	chromophore	UNP Q2MHN7
B	56	CR2	GLY	chromophore	UNP Q2MHN7
C	52	THR	HIS	engineered mutation	UNP Q2MHN7
C	56	CR2	GLY	chromophore	UNP Q2MHN7
C	56	CR2	TYR	chromophore	UNP Q2MHN7
C	56	CR2	GLY	chromophore	UNP Q2MHN7
D	52	THR	HIS	engineered mutation	UNP Q2MHN7
D	56	CR2	GLY	chromophore	UNP Q2MHN7
D	56	CR2	TYR	chromophore	UNP Q2MHN7
D	56	CR2	GLY	chromophore	UNP Q2MHN7

- Molecule 2 is 3-CYCLOHEXYL-1-PROPYLSULFONIC ACID (three-letter code: CXS) (formula: C₉H₁₉NO₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			14	9	1	3	1		
2	B	1	Total	C	N	O	S	0	0
			14	9	1	3	1		
2	B	1	Total	C	N	O	S	0	0
			14	9	1	3	1		
2	B	1	Total	C	N	O	S	0	0
			14	9	1	3	1		
2	D	1	Total	C	N	O	S	0	0
			14	9	1	3	1		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Cl	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	136	Total	O	0	0
			136	136		
4	B	126	Total	O	0	0
			126	126		
4	C	101	Total	O	0	0
			101	101		

Continued on next page...

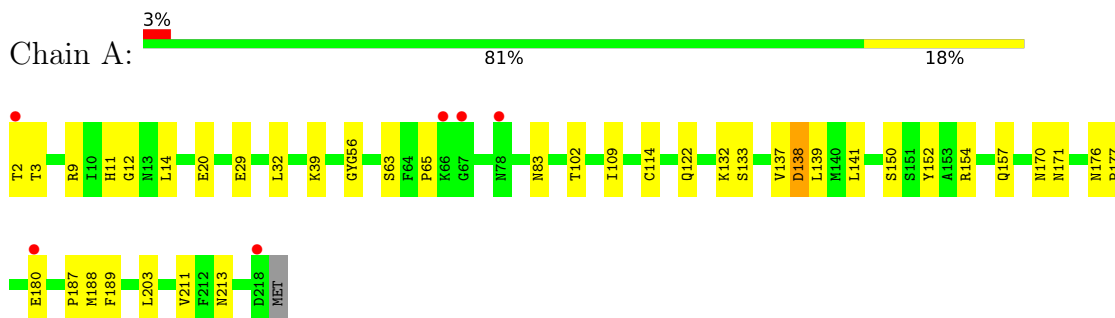
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	126	Total 126	O 126	0	0

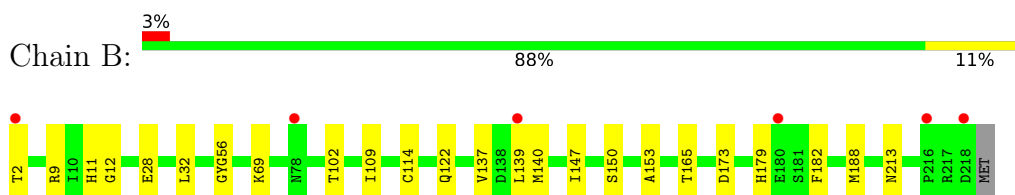
3 Residue-property plots [i](#)

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

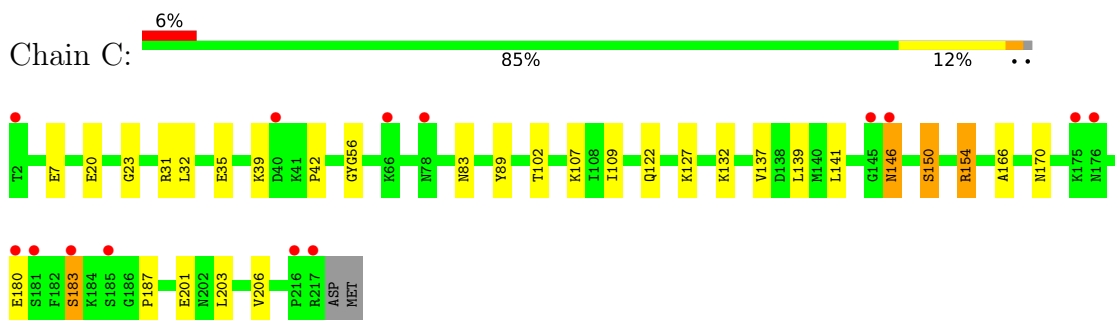
- Molecule 1: green fluorescent protein



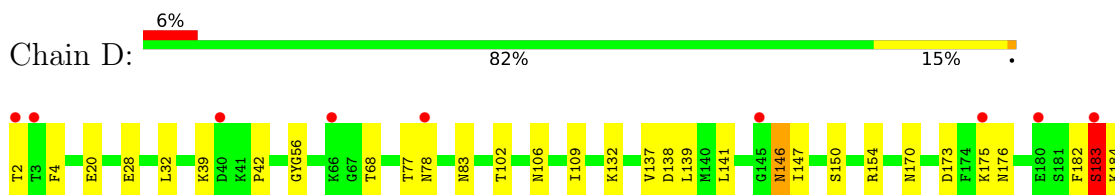
- Molecule 1: green fluorescent protein

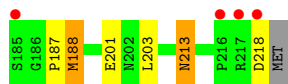


- Molecule 1: green fluorescent protein



- Molecule 1: green fluorescent protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	108.75Å 113.99Å 133.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.81 – 2.30 35.06 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.81-2.30) 100.0 (35.06-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.55 (at 2.29Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.185 , 0.218 0.178 , 0.182	Depositor DCC
R_{free} test set	3737 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	19.6	Xtrriage
Anisotropy	0.180	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 53.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.000 for k,h,-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7436	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.99 % 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 6.8915e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, CR2, CXS

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	0/1743	0.70	0/2347
1	B	0.48	0/1743	0.69	0/2347
1	C	0.44	0/1735	0.69	0/2336
1	D	0.45	0/1743	0.69	0/2347
All	All	0.46	0/6964	0.69	0/9377

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	1721	0	1663	28	0
1	B	1721	0	1663	17	0
1	C	1713	0	1659	20	0
1	D	1721	0	1663	30	1
2	A	14	0	19	2	0
2	B	42	0	57	2	0
2	D	14	0	19	0	0
3	B	1	0	0	0	0
4	A	136	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	126	0	0	1	1
4	C	101	0	0	0	0
4	D	126	0	0	3	0
All	All	7436	0	6743	93	1

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 7.

All (93) 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:A:137:VAL:HG11	1:B:137:VAL:HG11	1.63	0.81
1:C:7:GLU:HG3	1:C:107:LYS:HD2	1.68	0.76
1:B:2:THR:O	1:B:28:GLU:HA	1.90	0.72
1:C:137:VAL:HG11	1:D:137:VAL:HG11	1.73	0.70
1:D:146:ASN:H	1:D:146:ASN:HD22	1.37	0.70
1:B:139:LEU:HD23	1:B:140:MET:N	2.08	0.68
1:A:138:ASP:HB2	1:A:152:TYR:CD2	2.31	0.66
1:A:20:GLU:OE2	1:A:39:LYS:HE2	1.97	0.65
1:C:146:ASN:H	1:C:146:ASN:HD22	1.44	0.64
1:C:154:ARG:HH11	1:C:154:ARG:HB2	1.62	0.64
1:A:139:LEU:HD11	1:A:187:PRO:HB2	1.80	0.64
1:A:141:LEU:HD23	1:A:187:PRO:HB3	1.80	0.63
1:B:139:LEU:HD23	1:B:139:LEU:C	2.19	0.63
1:A:139:LEU:HD11	1:A:187:PRO:CB	2.30	0.62
1:D:154:ARG:HH11	1:D:154:ARG:HG3	1.65	0.61
1:C:154:ARG:HB2	1:C:154:ARG:NH1	2.15	0.60
1:A:139:LEU:CD1	1:A:187:PRO:HB2	2.31	0.60
1:D:32:LEU:HD12	1:D:32:LEU:C	2.24	0.58
1:A:83:ASN:HD21	1:A:170:ASN:HB3	1.69	0.58
1:A:141:LEU:CD2	1:A:187:PRO:HB3	2.36	0.55
1:B:69:LYS:HD3	1:B:179:HIS:CD2	2.42	0.55
1:B:153:ALA:HB1	2:B:1001:CXS:H81	1.88	0.55
1:D:2:THR:O	1:D:28:GLU:HA	2.08	0.54
1:A:32:LEU:HD12	1:A:32:LEU:C	2.27	0.54
1:D:141:LEU:HD23	1:D:187:PRO:HB3	1.90	0.54
1:C:20:GLU:OE1	1:C:39:LYS:HD3	2.09	0.53
1:B:147:ILE:HD13	1:B:173:ASP:HA	1.91	0.52
1:D:139:LEU:O	1:D:150:SER:HA	2.10	0.52
1:B:165:THR:HB	2:B:1001:CXS:H82	1.92	0.51
1:D:147:ILE:HD13	1:D:173:ASP:HA	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:MET:CE	1:A:213:ASN:HB3	2.41	0.51
1:D:203:LEU:HD12	1:D:203:LEU:N	2.26	0.51
1:A:29:GLU:HG3	1:A:63:SER:HA	1.92	0.51
1:D:20:GLU:OE1	1:D:39:LYS:HD3	2.11	0.50
1:A:132:LYS:HE2	1:A:157:GLN:OE1	2.12	0.50
1:C:32:LEU:C	1:C:32:LEU:HD12	2.32	0.50
2:A:1003:CXS:H71	1:C:127:LYS:HA	1.93	0.50
1:C:154:ARG:HH11	1:C:154:ARG:CB	2.24	0.50
1:B:32:LEU:C	1:B:32:LEU:HD12	2.32	0.49
1:A:138:ASP:OD1	1:A:150:SER:HB2	2.13	0.49
1:D:77:THR:HG22	1:D:77:THR:O	2.12	0.48
1:A:9:ARG:NH1	1:A:11:HIS:CD2	2.81	0.48
1:A:65:PRO:HD3	1:A:211:VAL:O	2.13	0.48
1:B:122:GLN:NE2	4:B:1155:HOH:O	2.46	0.48
1:D:150:SER:OG	1:D:170:ASN:HB2	2.13	0.48
1:A:139:LEU:HD13	1:A:189:PHE:CE2	2.48	0.48
1:A:171:ASN:HB3	2:A:1003:CXS:H82	1.95	0.48
1:D:78:ASN:O	1:D:176:ASN:ND2	2.42	0.47
1:C:83:ASN:HD21	1:C:170:ASN:HB3	1.79	0.47
1:C:146:ASN:HD22	1:C:146:ASN:N	2.08	0.47
1:A:133:SER:HB3	1:A:154:ARG:NH2	2.30	0.47
1:D:182:PHE:O	1:D:184:LYS:HD3	2.15	0.47
1:D:146:ASN:HD22	1:D:146:ASN:N	2.05	0.47
1:C:203:LEU:N	1:C:203:LEU:HD12	2.29	0.46
1:C:122:GLN:HE22	1:C:127:LYS:HZ1	1.63	0.46
1:A:12:GLY:HA3	1:A:114:CYS:O	2.16	0.46
1:B:139:LEU:C	1:B:139:LEU:CD2	2.85	0.45
1:A:176:ASN:HB3	1:A:177:PRO:HD2	1.99	0.45
1:A:203:LEU:HD12	1:A:203:LEU:N	2.31	0.45
1:B:12:GLY:HA3	1:B:114:CYS:O	2.17	0.45
1:D:175:LYS:O	1:D:175:LYS:HD3	2.17	0.45
1:D:213:ASN:HD22	1:D:213:ASN:C	2.20	0.45
1:D:83:ASN:HD21	1:D:170:ASN:HB3	1.82	0.45
1:C:141:LEU:HD23	1:C:187:PRO:HB3	1.98	0.44
1:A:122:GLN:NE2	4:A:1363:HOH:O	2.49	0.44
1:A:138:ASP:HA	1:A:152:TYR:HB3	1.99	0.44
1:D:102:THR:OG1	1:D:109:ILE:HB	2.17	0.44
1:D:42:PRO:HB3	1:D:201:GLU:HG2	2.00	0.44
1:A:102:THR:OG1	1:A:109:ILE:HB	2.18	0.44
1:A:188:MET:HE2	1:A:213:ASN:HB3	1.99	0.43
1:C:42:PRO:HB3	1:C:201:GLU:CG	2.47	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:THR:OG1	1:C:109:ILE:HB	2.18	0.43
1:D:138:ASP:OD1	1:D:150:SER:HB2	2.18	0.43
1:D:154:ARG:HG3	1:D:154:ARG:NH1	2.33	0.43
1:A:139:LEU:O	1:A:150:SER:HA	2.19	0.42
1:D:182:PHE:O	1:D:183:SER:C	2.57	0.42
1:C:89:TYR:CD2	1:C:166:ALA:HB2	2.54	0.42
1:C:139:LEU:O	1:C:150:SER:HA	2.20	0.42
1:B:9:ARG:NH1	1:B:11:HIS:CD2	2.88	0.42
1:D:102:THR:HG23	4:D:1138:HOH:O	2.19	0.42
1:D:154:ARG:NH1	4:D:1110:HOH:O	2.46	0.42
1:D:132:LYS:NZ	4:D:1481:HOH:O	2.50	0.42
1:A:2:THR:HG23	1:A:3:THR:N	2.35	0.41
1:B:102:THR:OG1	1:B:109:ILE:HB	2.19	0.41
1:D:4:PHE:CD1	1:D:4:PHE:N	2.88	0.41
1:B:139:LEU:O	1:B:150:SER:HA	2.20	0.41
1:B:188:MET:HG2	1:B:213:ASN:HB3	2.03	0.41
1:D:42:PRO:HB3	1:D:201:GLU:CG	2.50	0.41
1:D:2:THR:O	1:D:28:GLU:HB2	2.21	0.41
1:D:68:THR:HG21	1:D:188:MET:HE3	2.02	0.40
1:B:182:PHE:CD1	1:B:188:MET:HE3	2.56	0.40
1:C:23:GLY:HA3	1:C:35:GLU:O	2.21	0.40
1:C:31:ARG:NH1	1:C:206:VAL:HG11	2.37	0.40

All (1) 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)
1:D:106:ASN:N	4:B:1467:HOH:O[2_574]	2.14	0.06

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	210/216 (97%)	204 (97%)	6 (3%)	0	100	100
1	B	210/216 (97%)	204 (97%)	6 (3%)	0	100	100
1	C	209/216 (97%)	202 (97%)	6 (3%)	1 (0%)	29	35
1	D	210/216 (97%)	203 (97%)	6 (3%)	1 (0%)	29	35
All	All	839/864 (97%)	813 (97%)	24 (3%)	2 (0%)	47	58

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	183	SER
1	D	183	SER

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	186/187 (100%)	183 (98%)	3 (2%)	62	78
1	B	186/187 (100%)	186 (100%)	0	100	100
1	C	185/187 (99%)	179 (97%)	6 (3%)	39	54
1	D	186/187 (100%)	181 (97%)	5 (3%)	44	61
All	All	743/748 (99%)	729 (98%)	14 (2%)	57	73

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LEU
1	A	138	ASP
1	A	180	GLU
1	C	132	LYS
1	C	146	ASN
1	C	150	SER
1	C	154	ARG
1	C	180	GLU
1	C	183	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	146	ASN
1	D	183	SER
1	D	188	MET
1	D	213	ASN
1	D	218	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	ASN
1	A	83	ASN
1	A	106	ASN
1	A	122	GLN
1	A	146	ASN
1	B	11	HIS
1	B	83	ASN
1	B	106	ASN
1	B	122	GLN
1	B	146	ASN
1	C	74	HIS
1	C	78	ASN
1	C	83	ASN
1	C	122	GLN
1	C	146	ASN
1	D	74	HIS
1	D	83	ASN
1	D	146	ASN
1	D	213	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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
1	CR2	D	56	1	20,20,21	2.49	7 (35%)	25,27,29	3.54	8 (32%)
1	CR2	A	56	1	20,20,21	2.24	6 (30%)	25,27,29	3.50	9 (36%)
1	CR2	C	56	1	20,20,21	2.45	7 (35%)	25,27,29	3.43	9 (36%)
1	CR2	B	56	1	20,20,21	2.46	8 (40%)	25,27,29	3.46	7 (28%)

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
1	CR2	D	56	1	-	0/6/25/26	0/2/2/2
1	CR2	A	56	1	-	0/6/25/26	0/2/2/2
1	CR2	C	56	1	-	0/6/25/26	0/2/2/2
1	CR2	B	56	1	-	0/6/25/26	0/2/2/2

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	56	CR2	CD2-CG2	4.76	1.48	1.39
1	B	56	CR2	OH-CZ	4.73	1.48	1.37
1	D	56	CR2	OH-CZ	4.67	1.47	1.37
1	D	56	CR2	CE1-CZ	4.62	1.47	1.38
1	C	56	CR2	OH-CZ	4.61	1.47	1.37
1	A	56	CR2	OH-CZ	4.56	1.47	1.37
1	B	56	CR2	CE1-CD1	4.49	1.46	1.38
1	C	56	CR2	CE1-CZ	4.40	1.47	1.38
1	C	56	CR2	CD2-CG2	4.39	1.48	1.39
1	C	56	CR2	C1-N2	4.26	1.40	1.32
1	A	56	CR2	CE1-CD1	4.26	1.46	1.38
1	C	56	CR2	CE1-CD1	4.21	1.46	1.38
1	D	56	CR2	CE1-CD1	4.13	1.46	1.38
1	B	56	CR2	C1-N2	4.11	1.39	1.32
1	B	56	CR2	CD2-CG2	4.05	1.47	1.39
1	B	56	CR2	CE1-CZ	3.96	1.46	1.38
1	A	56	CR2	CE1-CZ	3.93	1.46	1.38
1	D	56	CR2	C1-N2	3.82	1.39	1.32
1	A	56	CR2	CD2-CG2	3.74	1.46	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	56	CR2	C1-N2	3.40	1.38	1.32
1	B	56	CR2	CD1-CG2	2.94	1.45	1.39
1	D	56	CR2	CD1-CG2	2.85	1.45	1.39
1	A	56	CR2	CD1-CG2	2.61	1.44	1.39
1	C	56	CR2	CD1-CG2	2.51	1.44	1.39
1	C	56	CR2	CE2-CD2	2.32	1.43	1.38
1	B	56	CR2	CE2-CD2	2.18	1.42	1.38
1	D	56	CR2	CE2-CD2	2.12	1.42	1.38
1	B	56	CR2	CG2-CB2	2.05	1.50	1.46

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	56	CR2	C2-N3-C1	12.30	114.00	107.99
1	B	56	CR2	C2-N3-C1	12.25	113.97	107.99
1	A	56	CR2	C2-N3-C1	11.65	113.68	107.99
1	C	56	CR2	C2-N3-C1	11.06	113.39	107.99
1	C	56	CR2	O2-C2-CA2	-9.38	125.69	130.96
1	A	56	CR2	O2-C2-CA2	-9.18	125.81	130.96
1	D	56	CR2	O2-C2-CA2	-8.57	126.15	130.96
1	B	56	CR2	O2-C2-CA2	-8.36	126.27	130.96
1	A	56	CR2	C1-CA1-N1	-4.88	102.05	112.85
1	C	56	CR2	C1-CA1-N1	-4.88	102.06	112.85
1	B	56	CR2	C1-CA1-N1	-4.66	102.53	112.85
1	D	56	CR2	C1-CA1-N1	-4.64	102.59	112.85
1	A	56	CR2	O2-C2-N3	3.71	131.72	124.35
1	D	56	CR2	O2-C2-N3	3.65	131.61	124.35
1	C	56	CR2	O2-C2-N3	3.60	131.50	124.35
1	B	56	CR2	O2-C2-N3	3.41	131.12	124.35
1	D	56	CR2	CA3-N3-C1	-3.36	123.22	127.86
1	B	56	CR2	CA3-N3-C1	-3.24	123.38	127.86
1	C	56	CR2	O3-C3-CA3	-3.07	117.11	126.39
1	A	56	CR2	CA3-N3-C1	-3.07	123.62	127.86
1	C	56	CR2	CA3-N3-C1	-3.02	123.69	127.86
1	D	56	CR2	O3-C3-CA3	-2.96	117.45	126.39
1	A	56	CR2	O3-C3-CA3	-2.83	117.84	126.39
1	B	56	CR2	O3-C3-CA3	-2.71	118.20	126.39
1	D	56	CR2	N3-C1-N2	-2.53	108.72	111.76
1	B	56	CR2	N3-C1-N2	-2.49	108.77	111.76
1	A	56	CR2	N3-C1-N2	-2.48	108.78	111.76
1	D	56	CR2	CA2-C2-N3	-2.44	102.22	103.37
1	C	56	CR2	N3-C1-N2	-2.39	108.89	111.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	CR2	CA1-C1-N3	2.12	125.35	122.52
1	A	56	CR2	CE1-CD1-CG2	-2.09	118.52	121.25
1	C	56	CR2	CE1-CD1-CG2	-2.05	118.58	121.25
1	C	56	CR2	CA1-C1-N3	2.02	125.23	122.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 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
2	CXS	B	1001	-	14,14,14	0.94	1 (7%)	18,18,18	1.79	7 (38%)
2	CXS	A	1003	-	14,14,14	1.14	1 (7%)	18,18,18	1.74	7 (38%)
2	CXS	B	1002	-	14,14,14	1.19	1 (7%)	18,18,18	1.63	6 (33%)
2	CXS	D	1005	-	14,14,14	1.23	1 (7%)	18,18,18	1.62	6 (33%)
2	CXS	B	1004	-	14,14,14	1.13	1 (7%)	18,18,18	1.78	7 (38%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CXS	B	1001	-	-	2/8/16/16	0/1/1/1
2	CXS	A	1003	-	-	2/8/16/16	0/1/1/1
2	CXS	B	1002	-	-	0/8/16/16	0/1/1/1
2	CXS	D	1005	-	-	0/8/16/16	0/1/1/1
2	CXS	B	1004	-	-	2/8/16/16	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1005	CXS	C1-S	3.14	1.82	1.77
2	A	1003	CXS	C1-S	3.10	1.81	1.77
2	B	1002	CXS	C1-S	3.09	1.81	1.77
2	B	1004	CXS	C1-S	2.80	1.81	1.77
2	B	1001	CXS	C1-S	2.06	1.80	1.77

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1004	CXS	C3-N-C4	-3.97	106.35	114.14
2	A	1003	CXS	C3-N-C4	-3.76	106.75	114.14
2	B	1001	CXS	C3-N-C4	-3.56	107.15	114.14
2	B	1004	CXS	C2-C1-S	-3.22	108.31	113.25
2	D	1005	CXS	O2-S-C1	2.92	110.43	106.92
2	B	1002	CXS	O2-S-C1	2.76	110.24	106.92
2	B	1001	CXS	C2-C1-S	-2.71	109.09	113.25
2	A	1003	CXS	O2-S-C1	2.67	110.13	106.92
2	B	1001	CXS	O3-S-C1	-2.57	101.62	105.77
2	A	1003	CXS	C2-C1-S	-2.55	109.34	113.25
2	B	1002	CXS	C3-N-C4	-2.52	109.18	114.14
2	B	1001	CXS	O3-S-O1	-2.52	105.12	111.27
2	D	1005	CXS	C3-N-C4	-2.51	109.21	114.14
2	B	1002	CXS	O3-S-O1	-2.50	105.16	111.27
2	D	1005	CXS	C2-C1-S	-2.43	109.52	113.25
2	B	1001	CXS	O2-S-C1	2.43	109.84	106.92
2	D	1005	CXS	O3-S-O1	-2.33	105.59	111.27
2	B	1001	CXS	O1-S-C1	2.32	109.71	106.92
2	B	1004	CXS	O2-S-C1	2.31	109.69	106.92
2	A	1003	CXS	O3-S-C1	-2.28	102.08	105.77
2	B	1002	CXS	C2-C1-S	-2.28	109.75	113.25
2	B	1004	CXS	O3-S-O1	-2.28	105.70	111.27
2	B	1002	CXS	O3-S-C1	-2.26	102.11	105.77
2	D	1005	CXS	O3-S-C1	-2.26	102.12	105.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1003	CXS	O3-S-O1	-2.22	105.85	111.27
2	A	1003	CXS	O2-S-O1	2.21	121.60	113.95
2	B	1004	CXS	O2-S-O1	2.17	121.47	113.95
2	B	1002	CXS	O2-S-O1	2.16	121.42	113.95
2	B	1001	CXS	O2-S-O1	2.14	121.36	113.95
2	A	1003	CXS	O3-S-O2	-2.12	106.08	111.27
2	B	1004	CXS	O3-S-C1	-2.08	102.40	105.77
2	D	1005	CXS	O2-S-O1	2.07	121.11	113.95
2	B	1004	CXS	O1-S-C1	2.00	109.33	106.92

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1001	CXS	C9-C4-N-C3
2	B	1004	CXS	C9-C4-N-C3
2	A	1003	CXS	C5-C4-N-C3
2	A	1003	CXS	C9-C4-N-C3
2	B	1004	CXS	C5-C4-N-C3
2	B	1001	CXS	C5-C4-N-C3

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1001	CXS	2	0
2	A	1003	CXS	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, 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	214/216 (99%)	-0.19	6 (2%) 53 60	9, 18, 37, 66	0
1	B	214/216 (99%)	-0.19	6 (2%) 53 60	8, 18, 40, 70	0
1	C	213/216 (98%)	0.04	14 (6%) 18 23	10, 21, 46, 65	0
1	D	214/216 (99%)	0.11	13 (6%) 21 27	9, 22, 48, 79	0
All	All	855/864 (98%)	-0.06	39 (4%) 32 39	8, 20, 44, 79	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	218	ASP	8.9
1	B	218	ASP	7.5
1	B	2	THR	5.8
1	A	218	ASP	5.7
1	D	185	SER	4.8
1	D	180	GLU	4.6
1	C	145	GLY	4.3
1	D	2	THR	4.3
1	D	78	ASN	4.2
1	C	66	LYS	4.2
1	D	40	ASP	4.2
1	C	180	GLU	4.1
1	B	180	GLU	4.0
1	C	185	SER	3.9
1	C	183	SER	3.9
1	D	216	PRO	3.8
1	C	2	THR	3.6
1	D	145	GLY	3.5
1	D	183	SER	3.5
1	A	66	LYS	3.2
1	C	216	PRO	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	78	ASN	3.0
1	C	78	ASN	2.9
1	C	40	ASP	2.9
1	D	3	THR	2.8
1	C	217	ARG	2.6
1	A	180	GLU	2.6
1	D	175	LYS	2.6
1	C	146	ASN	2.5
1	D	217	ARG	2.3
1	D	66	LYS	2.3
1	A	67	GLY	2.3
1	C	175	LYS	2.2
1	B	139	LEU	2.2
1	B	216	PRO	2.1
1	C	181	SER	2.1
1	A	78	ASN	2.1
1	A	2	THR	2.0
1	C	176	ASN	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	CR2	C	56	19/20	0.97	0.15	12,15,17,18	0
1	CR2	D	56	19/20	0.97	0.14	10,14,16,17	0
1	CR2	A	56	19/20	0.98	0.15	9,11,16,17	0
1	CR2	B	56	19/20	0.98	0.15	9,12,17,18	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	CXS	B	1001	14/14	0.69	0.31	51,54,72,72	0
2	CXS	A	1003	14/14	0.90	0.18	49,53,54,55	0
2	CXS	B	1004	14/14	0.90	0.17	49,54,56,56	0
2	CXS	B	1002	14/14	0.92	0.14	18,22,34,38	0
2	CXS	D	1005	14/14	0.95	0.11	18,22,33,36	0
3	CL	B	1006	1/1	0.99	0.06	13,13,13,13	0

6.5 Other polymers [i](#)

There are no such residues in this entry.