Full wwPDB X-ray Structure Validation Report ⓘ

Oct 21, 2024 – 08:04 PM EDT

PDB ID	:	3EFZ
Title	:	Crystal Structure of a 14-3-3 protein from cryptosporidium parvum (cgd1_2980)
Authors	:	Wernimont, A.K.; Dong, A.; Qiu, W.; Lew, J.; Wasney, G.A.; Vedadi, M.; Kozieradzki, I.; Zhao, Y.; Ren, H.; Alam, Z.; Lin, Y.H.; Sundstrom, M.; Weigelt, J.; Arrowsmith, C.H.; Edwards, A.M.; Bochkarev, A.; Hui, R.; Brokx, S.; Structural Genomics Consortium (SGC)
Deposited on	:	2008-09-10
Resolution	:	2.08 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

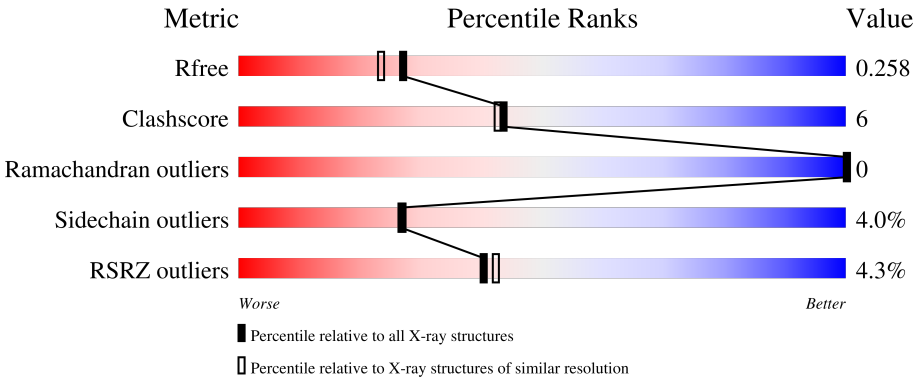
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)

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 2.08 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}	164625	7574 (2.10-2.06)
Clashscore	180529	8325 (2.10-2.06)
Ramachandran outliers	177936	8271 (2.10-2.06)
Sidechain outliers	177891	8272 (2.10-2.06)
RSRZ outliers	164620	7574 (2.10-2.06)

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 <=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	268	67% 12% 19%
1	B	268	6% 70% 12% 16%
1	C	268	3% 70% 8% 20%
1	D	268	3% 71% 7% 20%

Validation Pipeline (wwPDB-VP) : 2.39

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	EDO	C	302	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7491 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 14-3-3 protein.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	A	216	Total C N O P S 1777 1121 305 343 1 7	0	4	0
1	B	225	Total C N O S 1834 1156 304 369 5	0	4	0
1	C	214	Total C N O P S 1727 1089 295 336 1 6	0	2	0
1	D	214	Total C N O S 1709 1084 285 335 5	0	5	0

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP Q5CSF3
A	2	GLY	-	expression tag	UNP Q5CSF3
A	3	SER	-	expression tag	UNP Q5CSF3
A	4	SER	-	expression tag	UNP Q5CSF3
A	5	HIS	-	expression tag	UNP Q5CSF3
A	6	HIS	-	expression tag	UNP Q5CSF3
A	7	HIS	-	expression tag	UNP Q5CSF3
A	8	HIS	-	expression tag	UNP Q5CSF3
A	9	HIS	-	expression tag	UNP Q5CSF3
A	10	HIS	-	expression tag	UNP Q5CSF3
A	11	SER	-	expression tag	UNP Q5CSF3
A	12	SER	-	expression tag	UNP Q5CSF3
A	13	GLY	-	expression tag	UNP Q5CSF3
A	14	ARG	-	expression tag	UNP Q5CSF3
A	15	GLU	-	expression tag	UNP Q5CSF3
A	16	ASN	-	expression tag	UNP Q5CSF3
A	17	LEU	-	expression tag	UNP Q5CSF3
A	18	TYR	-	expression tag	UNP Q5CSF3
A	19	PHE	-	expression tag	UNP Q5CSF3
A	20	GLN	-	expression tag	UNP Q5CSF3
A	21	GLY	-	expression tag	UNP Q5CSF3

Continued on next page...

Continued from previous page...

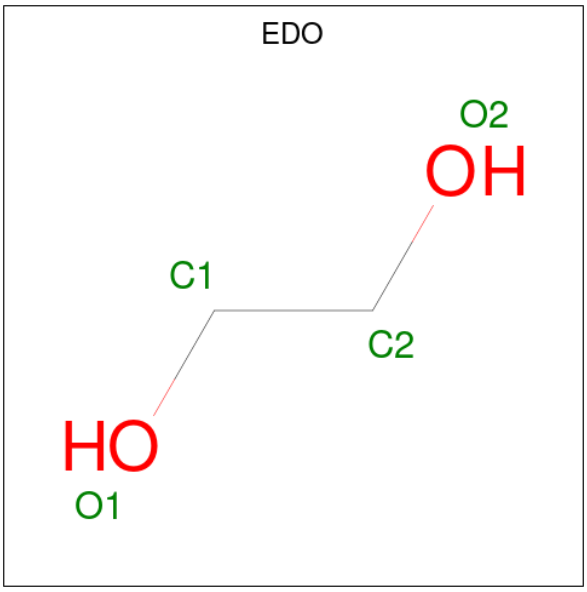
Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	expression tag	UNP Q5CSF3
B	2	GLY	-	expression tag	UNP Q5CSF3
B	3	SER	-	expression tag	UNP Q5CSF3
B	4	SER	-	expression tag	UNP Q5CSF3
B	5	HIS	-	expression tag	UNP Q5CSF3
B	6	HIS	-	expression tag	UNP Q5CSF3
B	7	HIS	-	expression tag	UNP Q5CSF3
B	8	HIS	-	expression tag	UNP Q5CSF3
B	9	HIS	-	expression tag	UNP Q5CSF3
B	10	HIS	-	expression tag	UNP Q5CSF3
B	11	SER	-	expression tag	UNP Q5CSF3
B	12	SER	-	expression tag	UNP Q5CSF3
B	13	GLY	-	expression tag	UNP Q5CSF3
B	14	ARG	-	expression tag	UNP Q5CSF3
B	15	GLU	-	expression tag	UNP Q5CSF3
B	16	ASN	-	expression tag	UNP Q5CSF3
B	17	LEU	-	expression tag	UNP Q5CSF3
B	18	TYR	-	expression tag	UNP Q5CSF3
B	19	PHE	-	expression tag	UNP Q5CSF3
B	20	GLN	-	expression tag	UNP Q5CSF3
B	21	GLY	-	expression tag	UNP Q5CSF3
C	1	MET	-	expression tag	UNP Q5CSF3
C	2	GLY	-	expression tag	UNP Q5CSF3
C	3	SER	-	expression tag	UNP Q5CSF3
C	4	SER	-	expression tag	UNP Q5CSF3
C	5	HIS	-	expression tag	UNP Q5CSF3
C	6	HIS	-	expression tag	UNP Q5CSF3
C	7	HIS	-	expression tag	UNP Q5CSF3
C	8	HIS	-	expression tag	UNP Q5CSF3
C	9	HIS	-	expression tag	UNP Q5CSF3
C	10	HIS	-	expression tag	UNP Q5CSF3
C	11	SER	-	expression tag	UNP Q5CSF3
C	12	SER	-	expression tag	UNP Q5CSF3
C	13	GLY	-	expression tag	UNP Q5CSF3
C	14	ARG	-	expression tag	UNP Q5CSF3
C	15	GLU	-	expression tag	UNP Q5CSF3
C	16	ASN	-	expression tag	UNP Q5CSF3
C	17	LEU	-	expression tag	UNP Q5CSF3
C	18	TYR	-	expression tag	UNP Q5CSF3
C	19	PHE	-	expression tag	UNP Q5CSF3
C	20	GLN	-	expression tag	UNP Q5CSF3
C	21	GLY	-	expression tag	UNP Q5CSF3

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	1	MET	-	expression tag	UNP Q5CSF3
D	2	GLY	-	expression tag	UNP Q5CSF3
D	3	SER	-	expression tag	UNP Q5CSF3
D	4	SER	-	expression tag	UNP Q5CSF3
D	5	HIS	-	expression tag	UNP Q5CSF3
D	6	HIS	-	expression tag	UNP Q5CSF3
D	7	HIS	-	expression tag	UNP Q5CSF3
D	8	HIS	-	expression tag	UNP Q5CSF3
D	9	HIS	-	expression tag	UNP Q5CSF3
D	10	HIS	-	expression tag	UNP Q5CSF3
D	11	SER	-	expression tag	UNP Q5CSF3
D	12	SER	-	expression tag	UNP Q5CSF3
D	13	GLY	-	expression tag	UNP Q5CSF3
D	14	ARG	-	expression tag	UNP Q5CSF3
D	15	GLU	-	expression tag	UNP Q5CSF3
D	16	ASN	-	expression tag	UNP Q5CSF3
D	17	LEU	-	expression tag	UNP Q5CSF3
D	18	TYR	-	expression tag	UNP Q5CSF3
D	19	PHE	-	expression tag	UNP Q5CSF3
D	20	GLN	-	expression tag	UNP Q5CSF3
D	21	GLY	-	expression tag	UNP Q5CSF3

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0

- Molecule 3 is water.

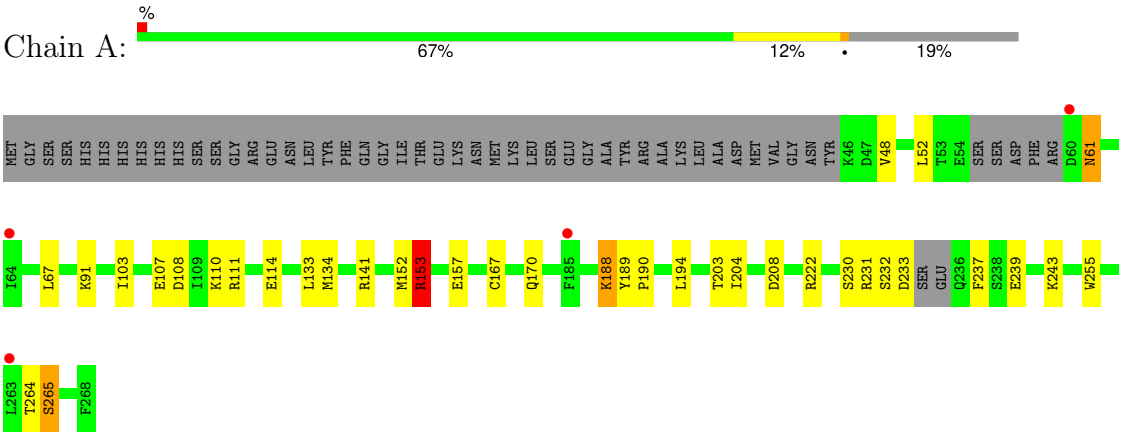
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	198	Total O 198 198	0	0
3	B	61	Total O 61 61	0	0
3	C	119	Total O 119 119	0	0
3	D	42	Total O 42 42	0	0

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.

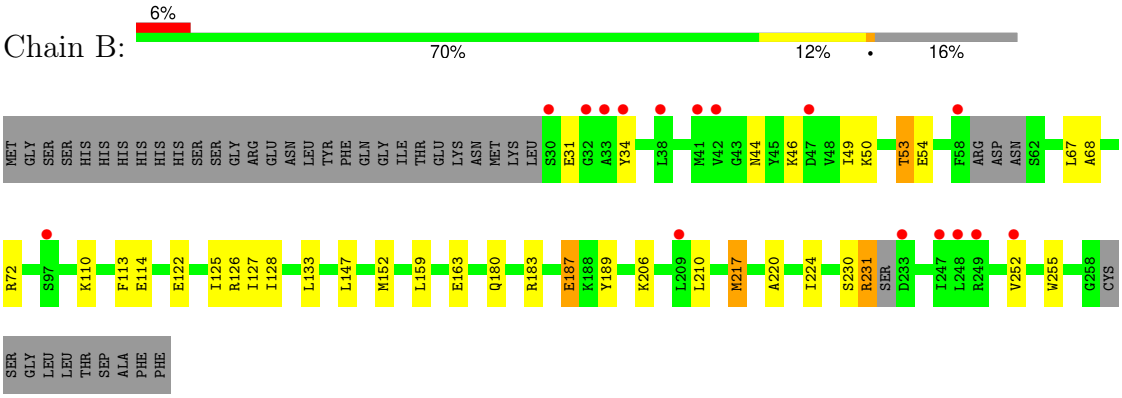
• Molecule 1: 14-3-3 protein

Chain A:



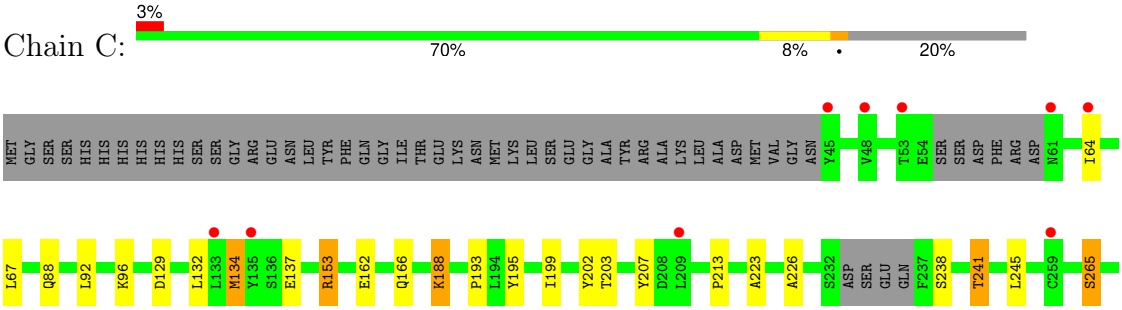
• Molecule 1: 14-3-3 protein

Chain B:



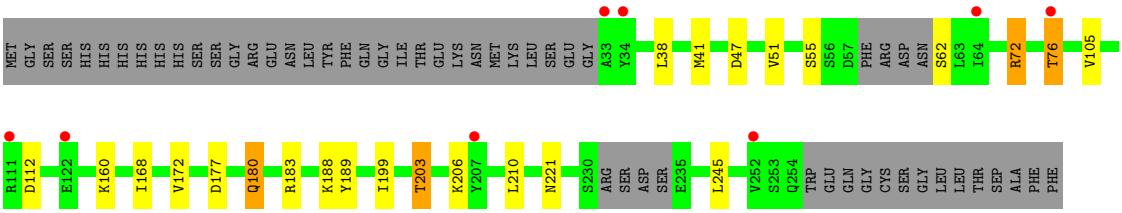
• Molecule 1: 14-3-3 protein

Chain C:



• Molecule 1: 14-3-3 protein

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	76.46Å 106.71Å 92.51Å 90.00° 112.83° 90.00°	Depositor
Resolution (Å)	25.00 – 2.08 25.00 – 2.08	Depositor EDS
% Data completeness (in resolution range)	99.3 (25.00-2.08) 99.2 (25.00-2.08)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	1.22 (at 2.08Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.225 , 0.267 0.222 , 0.258	Depositor DCC
R_{free} test set	4081 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	43.4	Xtriage
Anisotropy	0.004	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 42.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7491	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.79% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.58	0/1793	0.69	2/2397 (0.1%)
1	B	0.55	0/1865	0.64	0/2501
1	C	0.54	0/1736	0.67	2/2322 (0.1%)
1	D	0.52	0/1740	0.64	0/2338
All	All	0.55	0/7134	0.66	4/9558 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	153	ARG	NE-CZ-NH2	-10.64	114.98	120.30
1	A	153	ARG	NE-CZ-NH2	-9.37	115.61	120.30
1	A	153	ARG	NE-CZ-NH1	8.25	124.42	120.30
1	C	153	ARG	NE-CZ-NH1	6.62	123.61	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1777	0	1808	33	1
1	B	1834	0	1830	24	0
1	C	1727	0	1738	18	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1709	0	1700	12	0
2	A	4	0	6	0	0
2	B	4	0	6	1	0
2	C	12	0	18	4	0
2	D	4	0	6	0	0
3	A	198	0	0	3	0
3	B	61	0	0	1	1
3	C	119	0	0	2	0
3	D	42	0	0	1	0
All	All	7491	0	7112	85	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 6.

All (85) 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:152:MET:HE3	1:A:167:CYS:HA	1.48	0.96
1:A:152:MET:CE	1:A:167:CYS:HA	1.98	0.93
1:A:152:MET:HE2	1:A:170[A]:GLN:HB2	1.51	0.91
1:C:226:ALA:HB3	2:C:302:EDO:H12	1.60	0.84
1:B:159:LEU:HB3	1:B:163:GLU:HG3	1.60	0.84
1:D:72:ARG:O	1:D:76:THR:HG22	1.83	0.79
1:A:203:THR:HG22	1:A:255:TRP:HH2	1.47	0.77
1:C:153:ARG:NH2	1:C:265:SEP:O1P	2.17	0.77
1:D:199:ILE:O	1:D:203:THR:HG22	1.83	0.77
1:B:128:ILE:HD11	1:B:147:LEU:HD22	1.66	0.77
1:A:239:GLU:HG2	1:A:243:LYS:HE2	1.67	0.76
1:B:159:LEU:HB3	1:B:163:GLU:CG	2.17	0.74
1:C:188:LYS:HA	1:C:188:LYS:HE2	1.70	0.73
3:A:337:HOH:O	1:D:41:MET:HE1	1.88	0.72
1:B:49:ILE:O	1:B:53:THR:HB	1.89	0.71
1:C:134:MET:HE3	1:C:134:MET:H	1.54	0.71
1:A:153:ARG:NH2	1:A:265:SEP:O1P	2.24	0.71
1:A:152:MET:HE3	1:A:167:CYS:CA	2.20	0.70
1:B:230:SER:O	1:B:231:ARG:HG2	1.92	0.70
1:B:113:PHE:CD1	2:B:303:EDO:H11	2.29	0.67
1:A:152:MET:HE2	1:A:170[B]:GLN:HB2	1.76	0.67
1:B:187:GLU:H	1:B:187:GLU:CD	1.99	0.66
1:A:108:ASP:OD1	1:A:111:ARG:NH2	2.30	0.64
1:C:223:ALA:HA	2:C:302:EDO:H11	1.80	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:134:MET:H	1:C:134:MET:CE	2.11	0.63
1:A:232:SER:HA	1:A:233:ASP:C	2.20	0.62
1:C:162:GLU:O	1:C:166:GLN:HG3	1.99	0.61
1:B:180:GLN:OE1	1:B:183:ARG:NH1	2.36	0.59
1:D:51:VAL:O	1:D:55:SER:HB2	2.03	0.59
1:A:61:ASN:HD22	1:A:61:ASN:C	2.06	0.59
1:A:203:THR:HG22	1:A:255:TRP:CH2	2.34	0.58
1:A:203:THR:CG2	1:A:255:TRP:HH2	2.16	0.57
1:B:128:ILE:CD1	1:B:147:LEU:HD22	2.33	0.57
1:B:68:ALA:HB2	1:B:127:ILE:HG21	1.89	0.55
1:A:52:LEU:HD12	1:B:67:LEU:HD22	1.89	0.55
1:B:31:GLU:HB3	1:B:34:TYR:HB2	1.89	0.55
1:A:188:LYS:HE3	1:A:230:SER:HB2	1.89	0.55
1:B:53:THR:HG22	1:B:54:GLU:HG3	1.91	0.53
1:A:61:ASN:C	1:A:61:ASN:ND2	2.61	0.52
1:D:183:ARG:HG2	1:D:189:TYR:CE1	2.45	0.52
1:C:64:ILE:HG23	1:C:132:LEU:HD22	1.92	0.52
1:A:203:THR:CG2	1:A:255:TRP:CH2	2.93	0.51
1:C:195:TYR:CE2	2:C:302:EDO:H22	2.46	0.50
1:C:193:PRO:HG3	1:C:241:THR:HG22	1.93	0.50
1:A:231:ARG:HA	1:A:237:PHE:CZ	2.46	0.50
1:B:217:MET:HG3	1:B:252:VAL:HA	1.93	0.50
1:B:44:ASN:OD1	3:B:310:HOH:O	2.20	0.50
3:A:372:HOH:O	1:D:112:ASP:HB3	2.11	0.49
1:B:220:ALA:O	1:B:224:ILE:HG13	2.12	0.49
1:B:122[A]:GLU:HG3	1:B:126:ARG:CZ	2.43	0.48
1:C:223:ALA:HA	2:C:302:EDO:C1	2.43	0.48
1:B:230:SER:O	1:B:231:ARG:CG	2.61	0.48
1:C:199:ILE:O	1:C:203:THR:HG23	2.14	0.47
1:A:103:ILE:O	1:A:107:GLU:HG2	2.14	0.47
1:A:204:ILE:HD13	1:A:265:SEP:HB2	1.95	0.47
1:B:206:LYS:HA	1:B:210:LEU:HB2	1.97	0.47
1:C:88:GLN:HG3	1:D:105:VAL:HG21	1.95	0.47
1:C:92:LEU:HD12	1:C:96:LYS:HD3	1.97	0.47
1:A:110:LYS:O	1:A:114:GLU:HG3	2.15	0.46
1:A:48:VAL:O	1:A:52:LEU:HG	2.16	0.46
1:D:168:ILE:O	1:D:172:VAL:HG23	2.16	0.46
1:A:222[B]:ARG:HD2	3:C:322:HOH:O	2.16	0.45
1:D:72:ARG:CZ	1:D:76:THR:HG21	2.45	0.45
1:A:133:LEU:HD22	1:A:141:ARG:HG3	1.98	0.45
1:B:110:LYS:O	1:B:114:GLU:HG3	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:206:LYS:HA	1:D:210:LEU:HB2	1.98	0.45
1:B:125:ILE:HD13	1:B:152:MET:CE	2.47	0.45
1:D:177:ASP:O	1:D:180:GLN:HG3	2.17	0.45
1:A:153:ARG:O	1:A:157:GLU:HG3	2.18	0.44
1:A:204:ILE:HD11	1:A:264:THR:O	2.18	0.44
1:C:153:ARG:HH22	1:C:265:SEP:P	2.40	0.44
1:A:153:ARG:HH22	1:A:265:SEP:P	2.41	0.43
1:B:183:ARG:HG2	1:B:189:TYR:CE1	2.54	0.43
1:A:152:MET:HE2	1:A:170[A]:GLN:CB	2.36	0.43
1:C:129:ASP:O	1:C:134:MET:HE1	2.19	0.43
1:A:189:TYR:N	1:A:190:PRO:CD	2.81	0.43
1:B:46:LYS:HE2	1:B:50:LYS:HD2	2.01	0.42
1:B:217:MET:HG2	1:B:255:TRP:CD1	2.54	0.42
1:A:188:LYS:NZ	1:A:188:LYS:HB3	2.34	0.42
1:D:160:LYS:NZ	3:D:330:HOH:O	2.52	0.41
1:A:208:ASP:HB3	3:A:314:HOH:O	2.20	0.41
1:A:188:LYS:CE	1:A:230:SER:HB2	2.50	0.41
1:C:207:TYR:CE1	1:C:213:PRO:HB3	2.56	0.41
1:C:199:ILE:HG21	1:C:223:ALA:CB	2.51	0.40
1:A:91:LYS:HE3	3:C:366:HOH:O	2.22	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:A:232:SER:O	3:B:348:HOH:O[1_455]	2.19	0.01

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	213/268 (80%)	209 (98%)	4 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	223/268 (83%)	219 (98%)	4 (2%)	0	100	100
1	C	209/268 (78%)	201 (96%)	8 (4%)	0	100	100
1	D	213/268 (80%)	210 (99%)	3 (1%)	0	100	100
All	All	858/1072 (80%)	839 (98%)	19 (2%)	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	195/239 (82%)	188 (96%)	7 (4%)	30	31
1	B	202/239 (84%)	196 (97%)	6 (3%)	36	38
1	C	185/239 (77%)	177 (96%)	8 (4%)	25	24
1	D	181/239 (76%)	170 (94%)	11 (6%)	15	13
All	All	763/956 (80%)	731 (96%)	32 (4%)	27	25

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	ASN
1	A	67	LEU
1	A	134[A]	MET
1	A	134[B]	MET
1	A	153	ARG
1	A	188	LYS
1	A	194	LEU
1	B	53	THR
1	B	72	ARG
1	B	133	LEU
1	B	187	GLU
1	B	217	MET
1	B	231	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	67	LEU
1	C	134	MET
1	C	137	GLU
1	C	188	LYS
1	C	202	TYR
1	C	238	SER
1	C	241	THR
1	C	245	LEU
1	D	38	LEU
1	D	47[A]	ASP
1	D	47[B]	ASP
1	D	62	SER
1	D	72	ARG
1	D	76	THR
1	D	180	GLN
1	D	188	LYS
1	D	203	THR
1	D	221	ASN
1	D	245	LEU

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

Mol	Chain	Res	Type
1	A	61	ASN
1	B	44	ASN
1	B	229	ASN
1	D	229	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)

2 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	SEP	C	265	1	8,9,10	1.74	2 (25%)	7,12,14	1.02	0
1	SEP	A	265	1	8,9,10	1.89	3 (37%)	7,12,14	1.23	1 (14%)

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	SEP	C	265	1	-	0/6/8/10	-
1	SEP	A	265	1	-	0/6/8/10	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	265	SEP	P-O1P	3.91	1.62	1.50
1	C	265	SEP	P-O1P	3.65	1.61	1.50
1	A	265	SEP	P-O3P	2.28	1.63	1.54
1	C	265	SEP	P-O2P	2.17	1.62	1.54
1	A	265	SEP	P-O2P	2.01	1.62	1.54

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	265	SEP	OG-CB-CA	2.10	110.19	108.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	265	SEP	2	0
1	A	265	SEP	3	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

6 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	EDO	B	303	-	3,3,3	0.85	0	2,2,2	0.50	0
2	EDO	C	300	-	3,3,3	0.43	0	2,2,2	0.46	0
2	EDO	A	305	-	3,3,3	0.36	0	2,2,2	0.44	0
2	EDO	D	301	-	3,3,3	0.50	0	2,2,2	0.56	0
2	EDO	C	304	-	3,3,3	0.52	0	2,2,2	0.22	0
2	EDO	C	302	-	3,3,3	0.35	0	2,2,2	0.51	0

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	EDO	B	303	-	-	0/1/1/1	-
2	EDO	C	300	-	-	1/1/1/1	-
2	EDO	A	305	-	-	0/1/1/1	-
2	EDO	D	301	-	-	0/1/1/1	-
2	EDO	C	304	-	-	0/1/1/1	-
2	EDO	C	302	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	302	EDO	O1-C1-C2-O2
2	C	300	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	303	EDO	1	0
2	C	302	EDO	4	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	215/268 (80%)	0.14	4 (1%)	66	67	17, 37, 42, 47	4 (1%)
1	B	225/268 (83%)	0.44	16 (7%)	23	25	22, 37, 42, 44	4 (1%)
1	C	213/268 (79%)	0.26	9 (4%)	41	43	18, 37, 42, 45	4 (1%)
1	D	214/268 (79%)	0.25	8 (3%)	45	47	22, 37, 41, 51	5 (2%)
All	All	867/1072 (80%)	0.28	37 (4%)	40	42	17, 37, 42, 51	17 (1%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	58	PHE	6.1
1	B	33	ALA	4.8
1	A	64	ILE	3.9
1	B	247	ILE	3.8
1	B	38	LEU	3.7
1	C	45	TYR	3.7
1	B	32	GLY	3.6
1	C	64	ILE	3.1
1	C	259	CYS	3.1
1	B	41	MET	3.1
1	C	48	VAL	2.9
1	B	30	SER	2.9
1	D	34	TYR	2.9
1	B	42	VAL	2.8
1	A	60	ASP	2.7
1	B	97	SER	2.7
1	B	233	ASP	2.7
1	C	133	LEU	2.6
1	B	248	LEU	2.5
1	C	209	LEU	2.5
1	B	34	TYR	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	249	ARG	2.5
1	B	209	LEU	2.5
1	C	135	TYR	2.5
1	D	207	TYR	2.4
1	D	252	VAL	2.3
1	D	64	ILE	2.3
1	C	61	ASN	2.3
1	D	33	ALA	2.3
1	A	185	PHE	2.1
1	A	263	LEU	2.1
1	D	111[A]	ARG	2.1
1	D	122[A]	GLU	2.1
1	B	252	VAL	2.1
1	D	76	THR	2.1
1	B	47	ASP	2.0
1	C	53	THR	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	SEP	C	265	10/11	0.87	0.10	35,38,38,41	1
1	SEP	A	265	10/11	0.90	0.09	35,38,38,41	1

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	EDO	B	303	4/4	0.75	0.20	35,39,40,44	0
2	EDO	C	304	4/4	0.79	0.15	66,67,67,68	0
2	EDO	C	302	4/4	0.89	0.28	50,53,53,54	0
2	EDO	A	305	4/4	0.91	0.09	57,58,59,59	0
2	EDO	C	300	4/4	0.93	0.17	52,53,54,54	0
2	EDO	D	301	4/4	0.95	0.09	40,42,43,44	0

6.5 Other polymers (i)

There are no such residues in this entry.