Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 04:52 PM EDT

PDB ID	:	1FJ8
Title	:	THE STRUCTURE OF BETA-KETOACYL-[ACYL CARRIER PROTEIN] SYNTHASE I IN COMPLEX WITH CERULENIN, IMPLICATIONS FOR DRUG DESIGN
Authors	:	Price, A.C.; Choi, K.; Heath, R.J.; Li, Z.; White, S.W.; Rock, C.O.
Deposited on	:	2000-08-07
Resolution	:	2.27 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 (i) 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 (i)) were used in the production of this report:

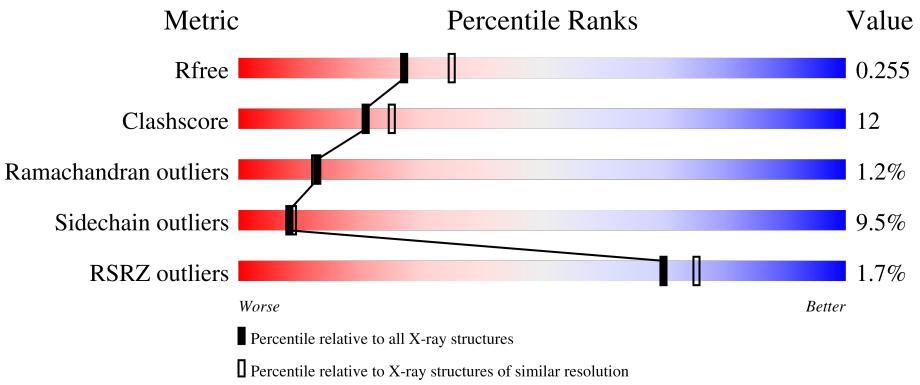
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.27 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	6980 (2.30-2.26)
Clashscore	141614	7711 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)
RSRZ outliers	127900	6849 (2.30-2.26)

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	406	2% 72% 23% 5% •
1	B	406	% 77% 19% • •
1	C	406	2% 74% 21% • •
1	D	406	2% 76% 18% 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	CER	A	500	-	-	X	-
2	CER	B	500	-	-	X	-
2	CER	C	500	-	-	X	-
2	CER	D	500	-	-	X	-

2 Entry composition (i)

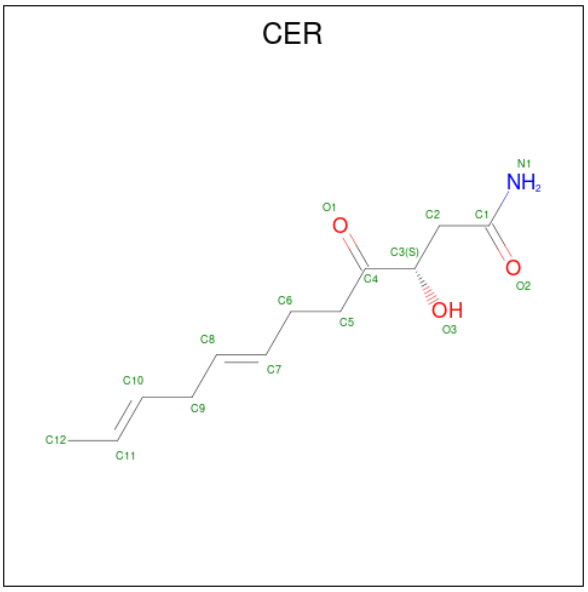
There are 3 unique types of molecules in this entry. The entry contains 12123 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 BETA-KETOACYL-[ACYL CARRIER PROTEIN] SYNTHASE I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	403	2955	1838	515	580	22	0	0	0
1	B	403	2955	1838	515	580	22	0	0	0
1	C	403	2955	1838	515	580	22	0	0	0
1	D	403	2955	1838	515	580	22	0	0	0

- Molecule 2 is (2S, 3R)-3-HYDROXY-4-OXO-7,10-TRANS,TRANS-DODECADIENAMIDE (three-letter code: CER) (formula: $C_{12}H_{19}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	16	12	1	3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	B	1	16	12	1	3	0	0
			Total	C	N	O		
2	C	1	16	12	1	3	0	0
			Total	C	N	O		
2	D	1	16	12	1	3	0	0

- Molecule 3 is water.

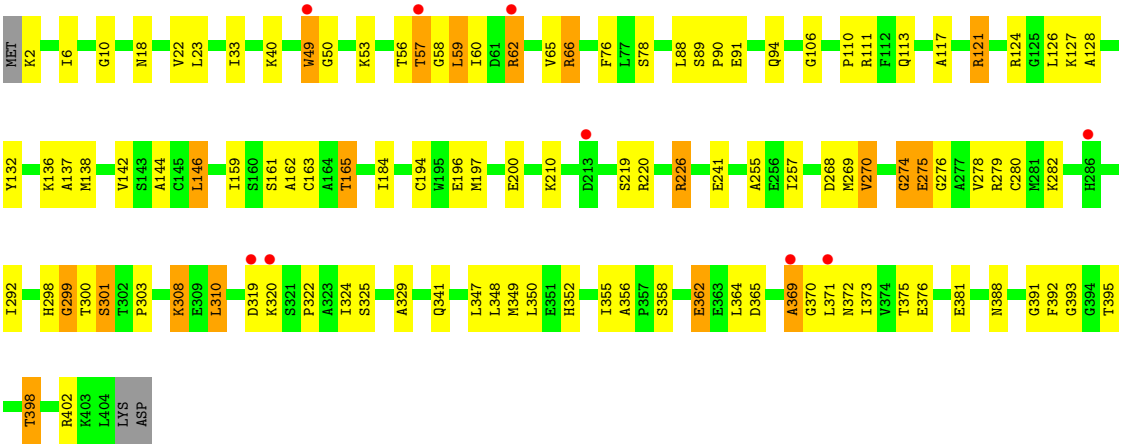
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	64	64	64	0	0
			Total	O		
3	B	61	61	61	0	0
			Total	O		
3	C	52	52	52	0	0
			Total	O		
3	D	62	62	62	0	0

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.

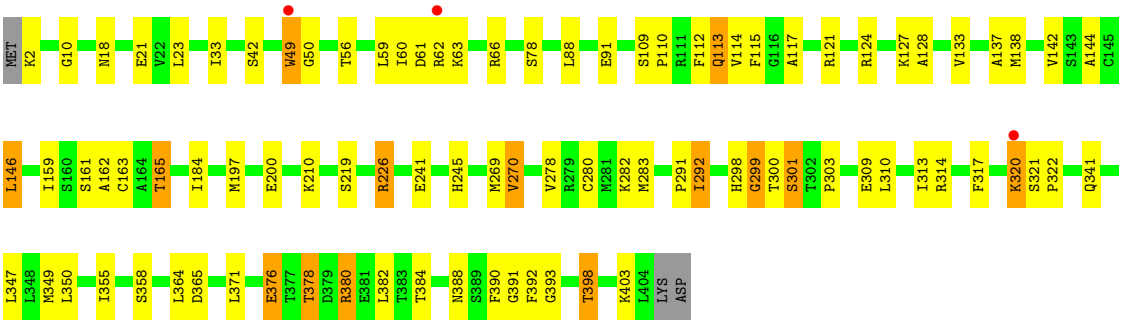
• Molecule 1: BETA-KETOACYL-[ACYL CARRIER PROTEIN] SYNTHASE I

Chain A:



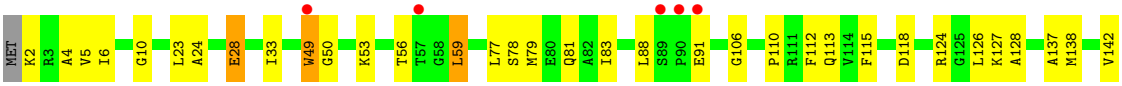
• Molecule 1: BETA-KETOACYL-[ACYL CARRIER PROTEIN] SYNTHASE I

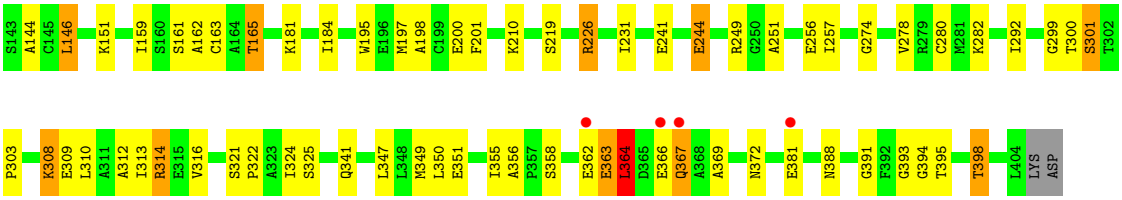
Chain B:



• Molecule 1: BETA-KETOACYL-[ACYL CARRIER PROTEIN] SYNTHASE I

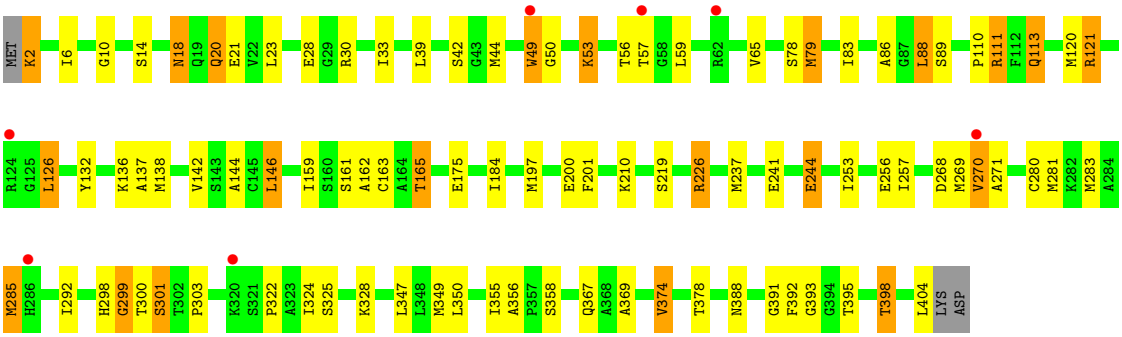
Chain C:





• Molecule 1: BETA-KETOACYL-[ACYL CARRIER PROTEIN] SYNTHASE I

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	59.23Å 139.59Å 212.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.27 19.89 – 2.27	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.27) 91.9 (19.89-2.27)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.03 (at 2.28Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.230 , 0.265 0.226 , 0.255	Depositor DCC
R_{free} test set	8004 reflections (10.03%)	wwPDB-VP
Wilson B-factor (Å^2)	19.0	Xtriage
Anisotropy	0.319	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 37.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	12123	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% 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 (i)

5.1 Standard geometry (i)

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

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	0.38	0/3003	0.64	1/4058 (0.0%)
1	B	0.39	0/3003	0.64	1/4058 (0.0%)
1	C	0.39	0/3003	0.64	1/4058 (0.0%)
1	D	0.38	0/3003	0.64	1/4058 (0.0%)
All	All	0.39	0/12012	0.64	4/16232 (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	B	50	GLY	N-CA-C	-5.67	98.93	113.10
1	A	50	GLY	N-CA-C	-5.58	99.14	113.10
1	D	50	GLY	N-CA-C	-5.50	99.36	113.10
1	C	50	GLY	N-CA-C	-5.46	99.44	113.10

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	2955	0	2909	74	0
1	B	2955	0	2909	69	0
1	C	2955	0	2909	75	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2955	0	2909	88	0
2	A	16	0	18	12	0
2	B	16	0	18	10	0
2	C	16	0	18	14	0
2	D	16	0	18	10	0
3	A	64	0	0	3	0
3	B	61	0	0	1	0
3	C	52	0	0	4	0
3	D	62	0	0	4	0
All	All	12123	0	11708	287	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 12.

All (287) 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:161:SER:H	1:A:165:THR:HG22	1.19	1.08
1:C:349:MET:HE3	1:C:355:ILE:HA	1.37	1.03
1:D:161:SER:H	1:D:165:THR:HG22	1.19	1.03
1:C:161:SER:H	1:C:165:THR:HG22	1.21	1.03
1:D:349:MET:HE3	1:D:355:ILE:HA	1.41	1.02
1:B:349:MET:HE3	1:B:355:ILE:HA	1.41	1.02
1:B:161:SER:H	1:B:165:THR:HG22	1.19	1.02
1:A:349:MET:HE3	1:A:355:ILE:HA	1.42	0.99
1:C:56:THR:HA	1:C:59:LEU:HD22	1.42	0.96
1:C:162:ALA:HB1	2:C:500:CER:H51	1.49	0.93
1:C:162:ALA:O	1:C:165:THR:HG23	1.72	0.89
1:D:162:ALA:O	1:D:165:THR:HG23	1.74	0.88
1:B:162:ALA:O	1:B:165:THR:HG23	1.73	0.88
1:C:198:ALA:HB1	3:C:509:HOH:O	1.73	0.87
1:A:162:ALA:O	1:A:165:THR:HG23	1.74	0.86
1:D:56:THR:HA	1:D:59:LEU:HD22	1.56	0.86
1:D:162:ALA:HB1	2:D:500:CER:H51	1.58	0.84
1:B:200:GLU:OE1	2:B:500:CER:H121	1.76	0.84
1:A:56:THR:HA	1:A:59:LEU:HD22	1.61	0.80
1:D:79:MET:HE2	1:D:83:ILE:HD11	1.64	0.79
1:C:113:GLN:HE21	1:D:110:PRO:HA	1.47	0.79
1:B:162:ALA:HB1	2:B:500:CER:H51	1.64	0.79
1:A:117:ALA:O	1:A:121:ARG:HD2	1.84	0.78
1:B:56:THR:HA	1:B:59:LEU:HD22	1.66	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:ARG:HB2	1:B:128:ALA:HB2	1.66	0.77
1:C:159:ILE:HD13	1:D:159:ILE:HD13	1.66	0.77
1:D:161:SER:N	1:D:165:THR:HG22	2.00	0.75
1:A:161:SER:N	1:A:165:THR:HG22	2.00	0.75
1:B:161:SER:N	1:B:165:THR:HG22	2.01	0.74
1:A:113:GLN:NE2	1:B:110:PRO:HA	2.01	0.74
1:A:159:ILE:HD13	1:B:159:ILE:HD13	1.68	0.73
1:C:231:ILE:HG21	3:C:509:HOH:O	1.89	0.73
1:D:18:ASN:ND2	1:D:21:GLU:H	1.87	0.72
1:D:355:ILE:HG21	1:D:374:VAL:HG11	1.70	0.72
1:A:162:ALA:HB1	2:A:500:CER:H51	1.69	0.72
1:A:269:MET:O	1:A:270:VAL:HG22	1.89	0.72
1:C:161:SER:N	1:C:165:THR:HG22	2.02	0.72
1:D:349:MET:CE	1:D:355:ILE:HA	2.18	0.72
1:B:241:GLU:OE1	1:B:245:HIS:HD2	1.74	0.71
1:C:184:ILE:HG12	1:C:241:GLU:HG3	1.70	0.71
1:B:269:MET:O	1:B:270:VAL:HG22	1.90	0.70
1:C:6:ILE:HD11	1:C:257:ILE:HD11	1.74	0.70
1:C:349:MET:CE	1:C:355:ILE:HA	2.18	0.70
1:A:162:ALA:HB1	2:A:500:CER:HO3	1.58	0.69
1:A:270:VAL:HA	1:A:392:PHE:CD1	2.27	0.69
2:A:500:CER:H101	1:B:138:MET:HA	1.75	0.69
1:A:349:MET:CE	1:A:355:ILE:HA	2.22	0.69
1:B:349:MET:CE	1:B:355:ILE:HA	2.20	0.69
1:C:118:ASP:CG	1:D:121:ARG:HH22	1.95	0.69
1:D:184:ILE:HG12	1:D:241:GLU:HG3	1.75	0.69
1:A:113:GLN:NE2	1:B:113:GLN:OE1	2.26	0.69
1:A:310:LEU:HG	1:A:371:LEU:CD1	2.23	0.68
1:B:63:LYS:O	1:B:66:ARG:HG2	1.93	0.68
1:C:118:ASP:OD1	1:D:121:ARG:NH2	2.27	0.68
1:A:6:ILE:HD11	1:A:257:ILE:HD11	1.75	0.67
1:B:184:ILE:HG12	1:B:241:GLU:HG3	1.77	0.66
1:C:110:PRO:HG2	1:C:197:MET:HB2	1.77	0.66
1:A:184:ILE:HG12	1:A:241:GLU:HG3	1.76	0.66
1:C:124:ARG:HB2	1:C:128:ALA:HB2	1.78	0.65
1:B:292:ILE:O	1:B:322:PRO:HB3	1.95	0.65
1:C:200:GLU:OE1	2:C:500:CER:H121	1.96	0.65
1:A:200:GLU:OE1	2:A:500:CER:H121	1.95	0.65
2:C:500:CER:H101	1:D:138:MET:HA	1.79	0.65
1:B:309:GLU:HG3	1:B:390:PHE:HE2	1.62	0.65
1:C:113:GLN:NE2	1:D:110:PRO:HA	2.12	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:308:LYS:HE3	1:C:308:LYS:HA	1.80	0.64
1:C:161:SER:H	1:C:165:THR:CG2	2.07	0.63
1:A:274:GLY:H	1:A:308:LYS:HE3	1.63	0.63
1:C:79:MET:O	1:C:83:ILE:HG13	1.99	0.63
1:B:127:LYS:HB2	1:B:127:LYS:NZ	2.14	0.62
1:A:110:PRO:HG2	1:A:197:MET:HB2	1.82	0.62
1:B:310:LEU:HD13	1:B:371:LEU:HD12	1.81	0.61
1:D:6:ILE:HD11	1:D:257:ILE:HD11	1.82	0.61
1:C:292:ILE:O	1:C:322:PRO:HB3	2.01	0.61
1:A:113:GLN:HE21	1:B:110:PRO:HA	1.64	0.61
1:A:200:GLU:HG2	1:B:133:VAL:HB	1.82	0.60
1:B:110:PRO:HG2	1:B:197:MET:HB2	1.83	0.60
1:A:348:LEU:O	1:A:352:HIS:HD2	1.86	0.59
1:B:270:VAL:HA	1:B:392:PHE:CD1	2.36	0.59
1:A:161:SER:H	1:A:165:THR:CG2	2.05	0.59
1:A:91:GLU:CD	1:A:91:GLU:H	2.06	0.58
1:C:124:ARG:HH11	1:C:127:LYS:HE3	1.69	0.58
1:B:226:ARG:NH1	1:B:303:PRO:HA	2.18	0.58
1:A:33:ILE:HA	1:A:49:TRP:O	2.04	0.58
1:B:388:ASN:OD1	1:B:398:THR:HB	2.04	0.57
1:A:56:THR:HA	1:A:59:LEU:CD2	2.33	0.57
1:A:226:ARG:NH1	1:A:303:PRO:HA	2.19	0.57
1:B:161:SER:H	1:B:165:THR:CG2	2.06	0.57
1:D:161:SER:H	1:D:165:THR:CG2	2.06	0.57
1:D:226:ARG:NH1	1:D:303:PRO:HA	2.20	0.56
1:D:244:GLU:OE1	1:D:244:GLU:HA	2.05	0.56
1:D:388:ASN:OD1	1:D:398:THR:HB	2.05	0.56
1:D:33:ILE:HA	1:D:49:TRP:O	2.05	0.56
1:D:200:GLU:OE1	2:D:500:CER:H121	2.06	0.56
1:A:226:ARG:NH2	1:A:365:ASP:OD1	2.38	0.56
1:B:33:ILE:HA	1:B:49:TRP:O	2.06	0.56
1:B:142:VAL:O	1:B:146:LEU:HG	2.05	0.56
1:A:142:VAL:O	1:A:146:LEU:HG	2.06	0.56
1:A:388:ASN:OD1	1:A:398:THR:HB	2.06	0.55
1:D:142:VAL:O	1:D:146:LEU:HG	2.06	0.55
1:B:392:PHE:H	2:B:500:CER:HO3	1.55	0.55
1:C:142:VAL:O	1:C:146:LEU:HG	2.06	0.55
1:C:388:ASN:OD1	1:C:398:THR:HB	2.07	0.55
1:C:363:GLU:O	1:C:364:LEU:CB	2.55	0.55
1:A:275:GLU:OE1	1:A:279:ARG:NH2	2.39	0.54
1:C:226:ARG:NH1	1:C:303:PRO:HA	2.22	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:33:ILE:HA	1:C:49:TRP:O	2.07	0.54
1:D:18:ASN:HD21	1:D:21:GLU:H	1.55	0.54
1:D:113:GLN:HE21	1:D:137:ALA:HB1	1.73	0.54
1:A:137:ALA:HB3	2:B:500:CER:H122	1.90	0.54
1:B:309:GLU:O	1:B:313:ILE:HG13	2.08	0.54
1:D:18:ASN:HD22	1:D:20:GLN:N	2.06	0.53
1:D:79:MET:HG2	1:D:237:MET:HG2	1.90	0.53
1:D:280:CYS:SG	1:D:398:THR:CG2	2.97	0.53
1:C:393:GLY:HA3	1:D:144:ALA:HB1	1.90	0.53
1:A:255:ALA:HB1	1:A:402:ARG:O	2.09	0.53
1:D:280:CYS:SG	1:D:398:THR:HG23	2.49	0.53
1:B:117:ALA:O	1:B:121:ARG:HD2	2.09	0.53
1:D:281:MET:O	1:D:285:MET:HG2	2.09	0.53
1:D:14:SER:O	1:D:53:LYS:NZ	2.41	0.53
1:D:292:ILE:O	1:D:322:PRO:HB3	2.09	0.53
1:D:18:ASN:HD21	1:D:20:GLN:HB3	1.75	0.52
1:B:391:GLY:HA2	2:B:500:CER:O3	2.10	0.52
1:C:341:GLN:NE2	3:C:535:HOH:O	2.42	0.52
1:B:162:ALA:HB1	2:B:500:CER:HO3	1.74	0.52
1:B:341:GLN:NE2	3:B:502:HOH:O	2.42	0.52
1:C:195:TRP:HA	1:C:198:ALA:HB3	1.89	0.52
1:C:197:MET:SD	2:C:500:CER:H91	2.50	0.52
1:C:280:CYS:SG	1:C:398:THR:CG2	2.98	0.52
1:A:310:LEU:HG	1:A:371:LEU:HD11	1.90	0.52
1:D:268:ASP:OD2	1:D:271:ALA:HB3	2.10	0.52
1:B:309:GLU:HG3	1:B:390:PHE:CE2	2.41	0.51
1:D:197:MET:SD	2:D:500:CER:H91	2.50	0.51
1:D:162:ALA:HB1	2:D:500:CER:HO3	1.75	0.51
1:D:269:MET:O	1:D:270:VAL:HG22	2.09	0.51
1:D:28:GLU:O	1:D:28:GLU:HG3	2.10	0.51
1:B:127:LYS:HB2	1:B:127:LYS:HZ3	1.76	0.51
1:D:18:ASN:HD22	1:D:18:ASN:C	2.14	0.51
1:A:197:MET:SD	2:A:500:CER:H91	2.51	0.51
1:B:226:ARG:NH2	1:B:365:ASP:OD1	2.43	0.51
1:C:138:MET:HA	2:D:500:CER:H101	1.91	0.51
1:C:201:PHE:HE2	2:C:500:CER:O1	1.94	0.51
1:C:24:ALA:O	1:C:28:GLU:HB2	2.11	0.50
1:B:163:CYS:SG	2:B:500:CER:H52	2.51	0.50
1:C:309:GLU:O	1:C:313:ILE:HG13	2.11	0.50
1:D:86:ALA:CB	1:D:88:LEU:HD22	2.41	0.50
1:B:117:ALA:O	1:B:121:ARG:CD	2.60	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:GLN:HE21	1:B:137:ALA:HB1	1.77	0.50
1:B:197:MET:SD	2:B:500:CER:H91	2.52	0.50
1:C:113:GLN:NE2	1:D:113:GLN:OE1	2.45	0.50
1:A:106:GLY:C	2:A:500:CER:H81	2.32	0.49
1:C:201:PHE:CE2	2:C:500:CER:O1	2.65	0.49
1:A:393:GLY:HA3	1:B:144:ALA:HB1	1.94	0.49
1:C:280:CYS:SG	1:C:398:THR:HG23	2.51	0.49
1:D:270:VAL:HA	1:D:392:PHE:CD1	2.47	0.49
1:C:300:THR:O	1:C:301:SER:HB3	2.12	0.49
1:C:274:GLY:O	1:C:278:VAL:HG23	2.13	0.49
1:D:163:CYS:SG	2:D:500:CER:H52	2.51	0.49
2:C:500:CER:C12	1:D:113:GLN:HE21	2.26	0.49
1:C:6:ILE:CD1	1:C:257:ILE:HD11	2.41	0.49
1:A:280:CYS:SG	1:A:398:THR:CG2	3.01	0.49
1:A:280:CYS:SG	1:A:398:THR:HG23	2.52	0.49
1:A:300:THR:O	1:A:301:SER:CB	2.60	0.48
1:A:369:ALA:O	1:A:371:LEU:N	2.39	0.48
1:D:79:MET:CE	1:D:83:ILE:HD11	2.40	0.48
2:A:500:CER:H122	1:B:137:ALA:CB	2.44	0.48
1:B:10:GLY:HA3	1:B:78:SER:O	2.12	0.48
1:D:391:GLY:HA2	2:D:500:CER:O3	2.14	0.48
1:B:300:THR:O	1:B:301:SER:CB	2.62	0.48
1:C:113:GLN:CD	1:D:113:GLN:OE1	2.52	0.48
1:D:18:ASN:ND2	1:D:20:GLN:HB3	2.28	0.48
1:A:292:ILE:O	1:A:322:PRO:HB3	2.14	0.48
1:C:163:CYS:SG	2:C:500:CER:H52	2.53	0.48
1:D:86:ALA:HB3	1:D:88:LEU:HD22	1.96	0.48
1:D:161:SER:OG	1:D:165:THR:HA	2.14	0.48
1:B:56:THR:O	1:B:59:LEU:HB2	2.14	0.47
1:D:10:GLY:HA3	1:D:78:SER:O	2.15	0.47
1:A:10:GLY:HA3	1:A:78:SER:O	2.14	0.47
1:C:144:ALA:HB1	1:D:393:GLY:HA3	1.97	0.47
1:C:162:ALA:O	1:C:165:THR:CG2	2.56	0.47
1:D:256:GLU:HB2	1:D:404:LEU:HD13	1.95	0.47
1:D:355:ILE:HB	1:D:378:THR:HG23	1.96	0.47
1:A:220:ARG:NH2	1:A:362:GLU:OE2	2.47	0.47
1:A:162:ALA:CB	2:A:500:CER:H51	2.44	0.47
1:A:124:ARG:HB2	1:A:128:ALA:HB2	1.97	0.47
1:A:138:MET:HA	2:B:500:CER:H101	1.96	0.47
1:A:275:GLU:HG3	1:A:276:GLY:N	2.31	0.46
1:C:10:GLY:HA3	1:C:78:SER:O	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:394:GLY:HA3	3:C:526:HOH:O	2.14	0.46
2:C:500:CER:H101	1:D:138:MET:CA	2.44	0.46
1:B:280:CYS:SG	1:B:398:THR:CG2	3.04	0.46
1:B:280:CYS:SG	1:B:398:THR:HG23	2.56	0.46
1:C:77:LEU:O	1:C:81:GLN:HG3	2.16	0.46
1:C:137:ALA:HB3	2:D:500:CER:H122	1.98	0.46
2:C:500:CER:H122	1:D:137:ALA:CB	2.46	0.46
1:D:283:MET:CE	3:D:534:HOH:O	2.64	0.46
1:D:2:LYS:HE2	1:D:2:LYS:HA	1.97	0.46
1:D:110:PRO:HG2	1:D:197:MET:HB2	1.99	0.45
1:C:391:GLY:HA2	2:C:500:CER:HO3	1.81	0.45
1:B:380:ARG:HG2	1:B:382:LEU:HD23	1.97	0.45
1:D:120:MET:HE1	1:D:126:LEU:HD13	1.97	0.45
1:B:161:SER:OG	1:B:165:THR:HA	2.16	0.45
1:A:348:LEU:O	1:A:352:HIS:CD2	2.66	0.45
1:A:341:GLN:NE2	3:A:547:HOH:O	2.49	0.45
2:A:500:CER:H122	1:B:137:ALA:HB3	1.99	0.45
1:B:162:ALA:CB	2:B:500:CER:H51	2.42	0.45
1:B:314:ARG:NH1	1:B:371:LEU:HD21	2.32	0.45
1:A:329:ALA:HB3	3:A:517:HOH:O	2.17	0.45
1:C:249:ARG:CZ	1:C:251:ALA:HB2	2.46	0.45
1:A:161:SER:OG	1:A:165:THR:HA	2.17	0.45
1:C:112:PHE:HA	1:C:115:PHE:HB3	1.99	0.44
1:A:375:THR:C	1:A:376:GLU:HG2	2.38	0.44
1:D:18:ASN:HD22	1:D:20:GLN:H	1.63	0.44
1:D:89:SER:HB3	3:D:518:HOH:O	2.16	0.44
1:A:163:CYS:SG	2:A:500:CER:H52	2.58	0.44
1:B:112:PHE:HA	1:B:115:PHE:HB3	1.99	0.44
1:A:300:THR:O	1:A:301:SER:HB3	2.17	0.44
1:B:109:SER:HB3	1:B:137:ALA:HA	2.00	0.43
1:C:106:GLY:O	2:C:500:CER:H81	2.18	0.43
1:D:269:MET:O	1:D:271:ALA:N	2.51	0.43
1:D:285:MET:HE2	1:D:285:MET:HA	1.99	0.43
1:B:162:ALA:O	1:B:165:THR:CG2	2.58	0.43
1:B:278:VAL:HG12	1:B:282:LYS:HD2	2.00	0.43
1:C:161:SER:OG	1:C:165:THR:HA	2.19	0.43
1:D:111:ARG:O	1:D:111:ARG:HG3	2.17	0.43
1:C:244:GLU:OE1	1:C:244:GLU:HA	2.19	0.43
1:C:181:LYS:NZ	1:D:175:GLU:OE2	2.41	0.43
1:D:395:THR:HG23	1:D:395:THR:O	2.18	0.43
1:A:362:GLU:H	1:A:362:GLU:HG2	1.41	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:PRO:O	1:B:114:VAL:HG23	2.19	0.42
1:B:226:ARG:NH1	1:B:303:PRO:O	2.48	0.42
1:C:162:ALA:CB	2:C:500:CER:H51	2.34	0.42
1:C:195:TRP:HH2	1:D:121:ARG:HD2	1.84	0.42
1:A:62:ARG:HH22	1:A:66:ARG:HB2	1.84	0.42
1:D:283:MET:HE1	3:D:534:HOH:O	2.19	0.42
1:A:60:ILE:HG12	1:A:76:PHE:CE1	2.54	0.42
1:C:124:ARG:NH1	1:C:127:LYS:HE3	2.33	0.42
1:A:57:THR:HG22	1:A:58:GLY:N	2.34	0.42
1:A:391:GLY:HA2	2:A:500:CER:O3	2.20	0.42
1:D:162:ALA:CB	2:D:500:CER:H51	2.40	0.42
1:C:278:VAL:HG12	1:C:282:LYS:HD2	2.01	0.42
1:C:349:MET:CE	1:C:356:ALA:H	2.32	0.42
1:D:253:ILE:HG21	1:D:404:LEU:HD22	2.01	0.42
1:D:324:ILE:HG22	1:D:325:SER:N	2.34	0.42
1:A:132:TYR:O	1:A:136:LYS:HG3	2.20	0.42
3:A:529:HOH:O	1:B:283:MET:CE	2.68	0.42
1:D:281:MET:O	1:D:285:MET:CG	2.67	0.42
1:A:194:CYS:HB2	1:A:196:GLU:OE1	2.20	0.42
1:A:278:VAL:HG12	1:A:282:LYS:HD2	2.02	0.42
1:A:324:ILE:HG22	1:A:325:SER:N	2.35	0.42
1:B:60:ILE:HG22	1:B:61:ASP:N	2.35	0.42
1:C:5:VAL:HG12	1:C:256:GLU:HB2	2.00	0.42
1:D:355:ILE:HG21	1:D:374:VAL:CG1	2.46	0.42
1:A:369:ALA:C	1:A:371:LEU:H	2.21	0.41
1:C:226:ARG:NH1	1:C:303:PRO:O	2.52	0.41
1:C:324:ILE:HG22	1:C:325:SER:N	2.35	0.41
1:D:300:THR:O	1:D:301:SER:CB	2.68	0.41
1:D:39:LEU:HD22	1:D:44:MET:SD	2.61	0.41
1:A:90:PRO:HA	1:A:94:GLN:HG3	2.02	0.41
1:C:300:THR:O	1:C:301:SER:CB	2.68	0.41
1:A:395:THR:HG23	1:A:395:THR:O	2.20	0.41
1:A:144:ALA:HB1	1:B:393:GLY:HA3	2.02	0.41
2:C:500:CER:H122	1:D:137:ALA:HB3	2.01	0.41
1:D:349:MET:CE	1:D:356:ALA:H	2.33	0.41
1:A:127:LYS:HB2	1:A:127:LYS:HE2	1.80	0.41
1:A:298:HIS:O	1:A:299:GLY:C	2.59	0.41
1:C:4:ALA:O	1:C:256:GLU:HG3	2.21	0.41
1:C:159:ILE:CD1	1:D:159:ILE:HD13	2.45	0.41
1:C:310:LEU:HD23	1:C:310:LEU:HA	1.95	0.41
1:D:201:PHE:HE2	2:D:500:CER:O1	2.04	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:226:ARG:NH1	1:D:303:PRO:O	2.48	0.41
1:D:298:HIS:O	1:D:299:GLY:C	2.58	0.41
1:D:328:LYS:HB2	3:D:521:HOH:O	2.20	0.41
1:B:18:ASN:OD1	1:B:21:GLU:HG3	2.21	0.41
1:B:376:GLU:O	1:B:378:THR:HG23	2.21	0.41
1:C:312:ALA:O	1:C:316:VAL:HG23	2.21	0.41
1:A:18:ASN:O	1:A:22:VAL:HG23	2.21	0.40
1:B:298:HIS:O	1:B:299:GLY:C	2.60	0.40
1:B:317:PHE:O	1:B:320:LYS:HG3	2.21	0.40
1:C:351:GLU:O	1:C:351:GLU:HG3	2.20	0.40
1:A:349:MET:CE	1:A:356:ALA:H	2.33	0.40
1:C:314:ARG:NH1	1:C:369:ALA:O	2.54	0.40
1:D:132:TYR:O	1:D:136:LYS:HG3	2.21	0.40
1:B:291:PRO:O	1:B:384:THR:HB	2.21	0.40
1:D:18:ASN:ND2	1:D:18:ASN:C	2.75	0.40
1:A:392:PHE:H	2:A:500:CER:HO3	1.70	0.40
1:C:395:THR:HG23	1:C:395:THR:O	2.22	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	401/406 (99%)	374 (93%)	19 (5%)	8 (2%)	7 5
1	B	401/406 (99%)	379 (94%)	19 (5%)	3 (1%)	22 25
1	C	401/406 (99%)	379 (94%)	18 (4%)	4 (1%)	15 16
1	D	401/406 (99%)	377 (94%)	19 (5%)	5 (1%)	13 12
All	All	1604/1624 (99%)	1509 (94%)	75 (5%)	20 (1%)	13 12

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	299	GLY
1	B	299	GLY
1	C	299	GLY
1	D	57	THR
1	D	270	VAL
1	D	299	GLY
1	D	369	ALA
1	A	57	THR
1	A	270	VAL
1	A	319	ASP
1	A	369	ALA
1	B	270	VAL
1	C	364	LEU
1	A	274	GLY
1	A	301	SER
1	A	370	GLY
1	B	301	SER
1	C	301	SER
1	C	367	GLN
1	D	301	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	306/309 (99%)	273 (89%)	33 (11%)	6 6
1	B	306/309 (99%)	281 (92%)	25 (8%)	11 13
1	C	306/309 (99%)	276 (90%)	30 (10%)	8 8
1	D	306/309 (99%)	278 (91%)	28 (9%)	9 10
All	All	1224/1236 (99%)	1108 (90%)	116 (10%)	8 9

All (116) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	23	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	40	LYS
1	A	49	TRP
1	A	53	LYS
1	A	59	LEU
1	A	62	ARG
1	A	65	VAL
1	A	66	ARG
1	A	88	LEU
1	A	89	SER
1	A	111	ARG
1	A	121	ARG
1	A	126	LEU
1	A	146	LEU
1	A	165	THR
1	A	210	LYS
1	A	219	SER
1	A	226	ARG
1	A	268	ASP
1	A	275	GLU
1	A	308	LYS
1	A	310	LEU
1	A	320	LYS
1	A	347	LEU
1	A	350	LEU
1	A	358	SER
1	A	362	GLU
1	A	364	LEU
1	A	372	ASN
1	A	373	ILE
1	A	381	GLU
1	A	398	THR
1	B	2	LYS
1	B	23	LEU
1	B	42	SER
1	B	49	TRP
1	B	62	ARG
1	B	88	LEU
1	B	91	GLU
1	B	113	GLN
1	B	146	LEU
1	B	165	THR
1	B	210	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	219	SER
1	B	226	ARG
1	B	292	ILE
1	B	320	LYS
1	B	321	SER
1	B	347	LEU
1	B	350	LEU
1	B	358	SER
1	B	364	LEU
1	B	376	GLU
1	B	378	THR
1	B	380	ARG
1	B	398	THR
1	B	403	LYS
1	C	2	LYS
1	C	23	LEU
1	C	28	GLU
1	C	49	TRP
1	C	53	LYS
1	C	59	LEU
1	C	88	LEU
1	C	91	GLU
1	C	126	LEU
1	C	146	LEU
1	C	151	LYS
1	C	165	THR
1	C	210	LYS
1	C	219	SER
1	C	226	ARG
1	C	244	GLU
1	C	308	LYS
1	C	314	ARG
1	C	321	SER
1	C	347	LEU
1	C	350	LEU
1	C	358	SER
1	C	362	GLU
1	C	363	GLU
1	C	364	LEU
1	C	366	GLU
1	C	367	GLN
1	C	372	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	381	GLU
1	C	398	THR
1	D	2	LYS
1	D	18	ASN
1	D	20	GLN
1	D	23	LEU
1	D	30	ARG
1	D	42	SER
1	D	49	TRP
1	D	53	LYS
1	D	65	VAL
1	D	79	MET
1	D	88	LEU
1	D	111	ARG
1	D	113	GLN
1	D	121	ARG
1	D	126	LEU
1	D	146	LEU
1	D	165	THR
1	D	210	LYS
1	D	219	SER
1	D	226	ARG
1	D	244	GLU
1	D	285	MET
1	D	347	LEU
1	D	350	LEU
1	D	358	SER
1	D	367	GLN
1	D	374	VAL
1	D	398	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	113	GLN
1	A	172	ASN
1	A	225	HIS
1	A	341	GLN
1	A	352	HIS
1	A	372	ASN
1	B	37	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	172	ASN
1	B	245	HIS
1	B	341	GLN
1	B	372	ASN
1	C	20	GLN
1	C	37	GLN
1	C	113	GLN
1	C	172	ASN
1	C	341	GLN
1	C	352	HIS
1	C	372	ASN
1	D	18	ASN
1	D	172	ASN
1	D	341	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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	CER	B	500	1	14,15,15	1.50	2 (14%)	13,17,17	1.10	0
2	CER	C	500	1	14,15,15	1.46	2 (14%)	13,17,17	1.09	0
2	CER	A	500	1	14,15,15	1.47	2 (14%)	13,17,17	1.11	0
2	CER	D	500	1	14,15,15	1.45	2 (14%)	13,17,17	1.09	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	CER	B	500	1	-	7/16/16/16	-
2	CER	C	500	1	-	7/16/16/16	-
2	CER	A	500	1	-	7/16/16/16	-
2	CER	D	500	1	-	7/16/16/16	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	CER	C8-C7	3.89	1.54	1.31
2	C	500	CER	C8-C7	3.87	1.54	1.31
2	A	500	CER	C8-C7	3.86	1.54	1.31
2	D	500	CER	C8-C7	3.84	1.54	1.31
2	A	500	CER	C10-C11	3.39	1.55	1.29
2	B	500	CER	C10-C11	3.38	1.54	1.29
2	D	500	CER	C10-C11	3.31	1.54	1.29
2	C	500	CER	C10-C11	3.23	1.53	1.29

There are no bond angle outliers.

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500	CER	C4-C5-C6-C7
2	A	500	CER	C9-C10-C11-C12
2	B	500	CER	C4-C5-C6-C7
2	B	500	CER	C9-C10-C11-C12
2	C	500	CER	C4-C5-C6-C7
2	C	500	CER	C9-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	D	500	CER	C4-C5-C6-C7
2	D	500	CER	C9-C10-C11-C12
2	A	500	CER	C6-C7-C8-C9
2	B	500	CER	C6-C7-C8-C9
2	C	500	CER	C6-C7-C8-C9
2	D	500	CER	C6-C7-C8-C9
2	B	500	CER	N1-C1-C2-C3
2	C	500	CER	N1-C1-C2-C3
2	D	500	CER	N1-C1-C2-C3
2	A	500	CER	O2-C1-C2-C3
2	D	500	CER	O2-C1-C2-C3
2	A	500	CER	C11-C10-C9-C8
2	B	500	CER	C11-C10-C9-C8
2	C	500	CER	C11-C10-C9-C8
2	D	500	CER	C11-C10-C9-C8
2	A	500	CER	N1-C1-C2-C3
2	B	500	CER	O2-C1-C2-C3
2	C	500	CER	O2-C1-C2-C3
2	C	500	CER	C5-C6-C7-C8
2	D	500	CER	C5-C6-C7-C8
2	A	500	CER	C5-C6-C7-C8
2	B	500	CER	C5-C6-C7-C8

There are no ring outliers.

4 monomers are involved in 46 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	500	CER	10	0
2	C	500	CER	14	0
2	A	500	CER	12	0
2	D	500	CER	10	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 (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	403/406 (99%)	0.15	9 (2%)	62	68	8, 19, 35, 45	0
1	B	403/406 (99%)	-0.07	3 (0%)	87	90	7, 16, 27, 40	0
1	C	403/406 (99%)	0.07	9 (2%)	62	68	9, 18, 30, 49	0
1	D	403/406 (99%)	-0.03	7 (1%)	70	75	5, 17, 30, 43	0
All	All	1612/1624 (99%)	0.03	28 (1%)	70	75	5, 17, 31, 49	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	366	GLU	4.9
1	A	319	ASP	3.7
1	A	49	TRP	3.4
1	D	286	HIS	3.4
1	C	362	GLU	3.3
1	A	369	ALA	3.0
1	C	89	SER	3.0
1	A	286	HIS	2.8
1	D	62	ARG	2.8
1	A	320	LYS	2.7
1	C	90	PRO	2.6
1	A	57	THR	2.6
1	D	270	VAL	2.6
1	B	320	LYS	2.6
1	A	213	ASP	2.6
1	B	62	ARG	2.5
1	C	367	GLN	2.5
1	D	57	THR	2.3
1	D	320	LYS	2.3
1	C	57	THR	2.2
1	D	124	ARG	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	62	ARG	2.2
1	B	49	TRP	2.2
1	D	49	TRP	2.1
1	C	91	GLU	2.1
1	A	371	LEU	2.1
1	C	381	GLU	2.1
1	C	49	TRP	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 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(Å^2)	Q<0.9
2	CER	B	500	16/16	0.69	0.36	38,40,43,43	0
2	CER	C	500	16/16	0.74	0.34	38,40,43,43	0
2	CER	D	500	16/16	0.76	0.36	38,40,43,43	0
2	CER	A	500	16/16	0.80	0.31	38,40,43,43	0

6.5 Other polymers (i)

There are no such residues in this entry.