



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:50 AM UTC

PDB ID : 1J11 / pdb_00001j11
Title : beta-amylase from *Bacillus cereus* var. *mycoides* in complex with alpha-EPG
Authors : Oyama, T.; Miyake, H.; Kusunoki, M.; Nitta, Y.
Deposited on : 2002-11-25
Resolution : 2.00 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

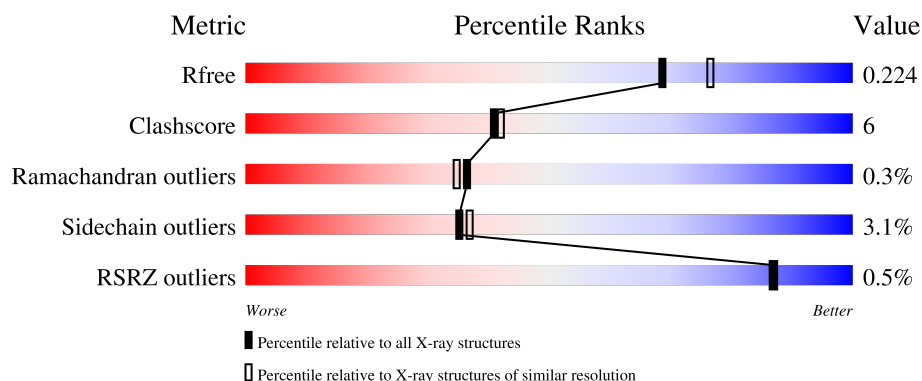
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	516	 82% 16% .
1	B	516	 78% 21% .
1	C	516	 80% 17% .
1	D	516	 78% 20% .

2 Entry composition [i](#)

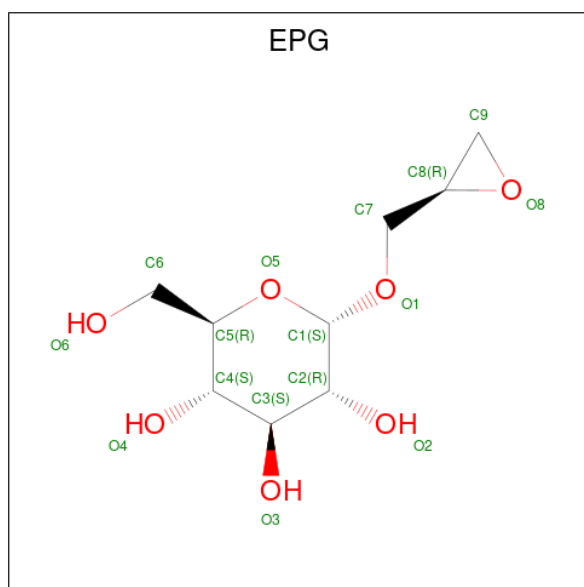
There are 4 unique types of molecules in this entry. The entry contains 17070 atoms, of which 0 are hydrogens and 0 are deuteriums.

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-amylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	516	Total	C	N	O	S	0	0	0
			4119	2645	676	781	17			
1	B	516	Total	C	N	O	S	0	0	0
			4119	2645	676	781	17			
1	C	516	Total	C	N	O	S	0	0	0
			4119	2645	676	781	17			
1	D	516	Total	C	N	O	S	0	0	0
			4119	2645	676	781	17			

- Molecule 2 is (2R)-oxiran-2-ylmethyl alpha-D-glucopyranoside (CCD ID: EPG) (formula: C₉H₁₆O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			16	9	7		
2	B	1	Total	C	O	0	0
			16	9	7		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			16	9	7		
2	D	1	Total	C	O	0	0
			16	9	7		

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		
3	B	1	Total	Ca	0	0
			1	1		
3	C	1	Total	Ca	0	0
			1	1		
3	D	1	Total	Ca	0	0
			1	1		

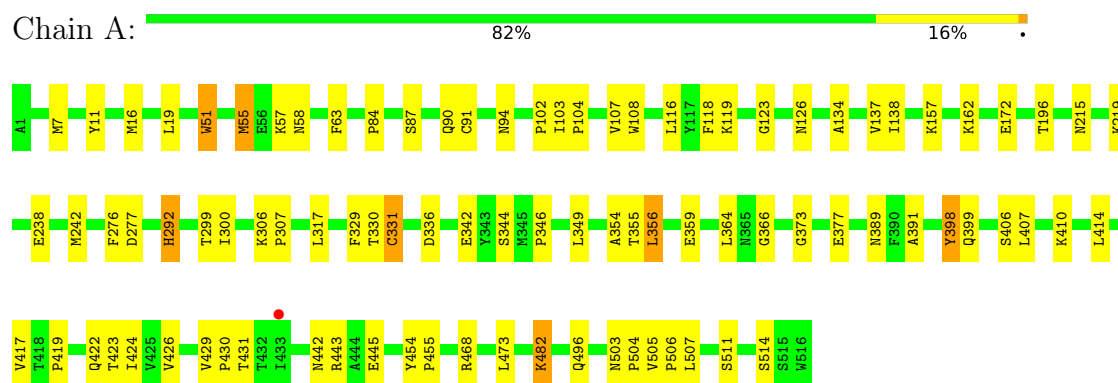
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	160	Total	O	0	0
			160	160		
4	B	103	Total	O	0	0
			103	103		
4	C	138	Total	O	0	0
			138	138		
4	D	125	Total	O	0	0
			125	125		

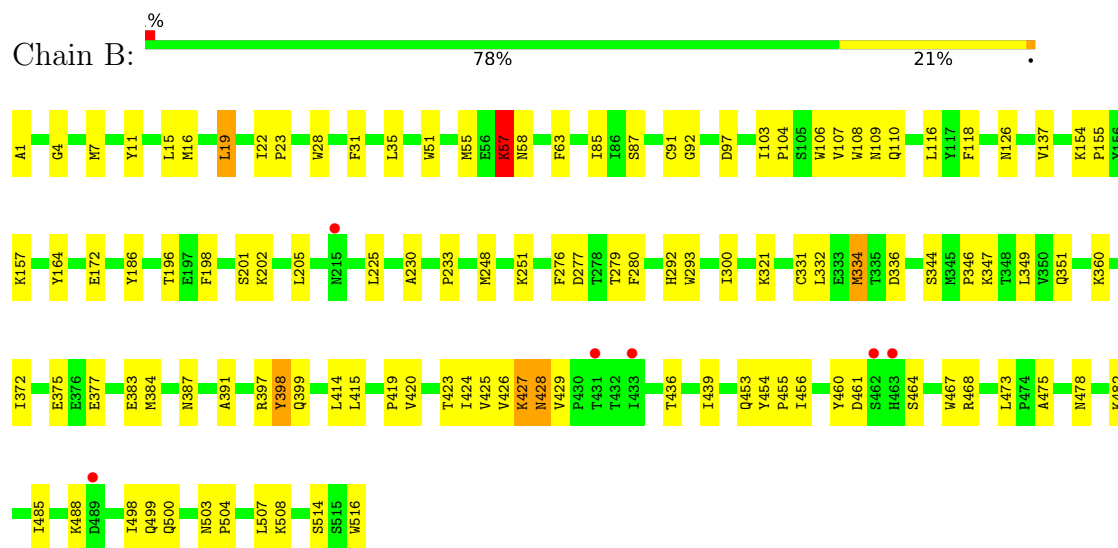
3 Residue-property plots

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.

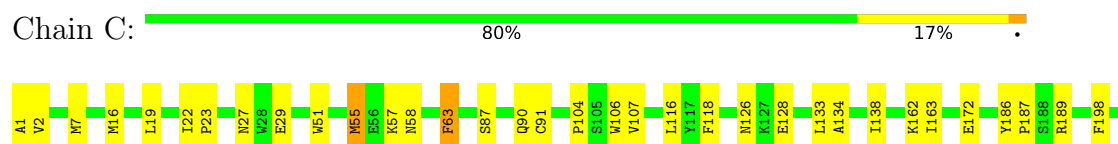
• Molecule 1: Beta-amylase

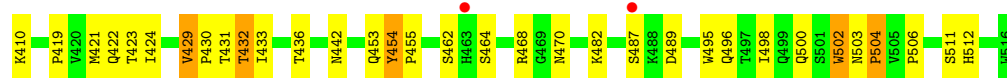


• Molecule 1: Beta-amylase

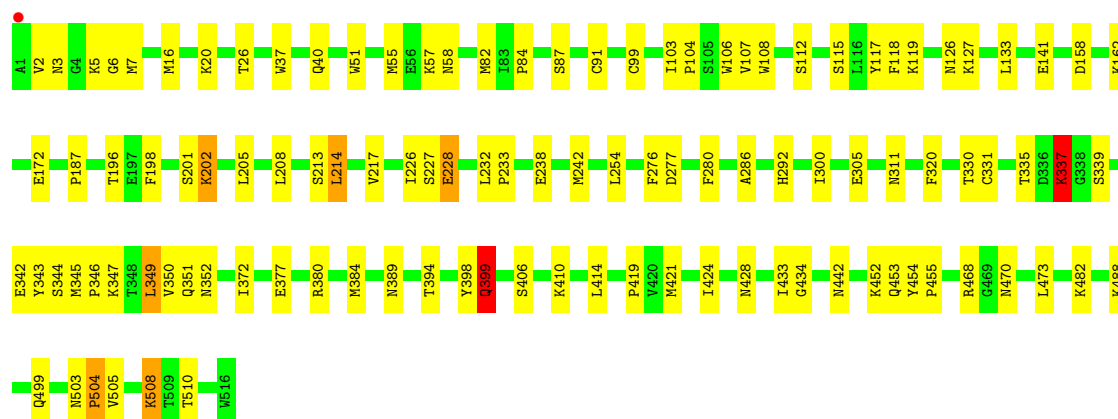


• Molecule 1: Beta-amylase





Chain D: 78% 20%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	177.90Å 112.90Å 146.20Å 90.00° 105.80° 90.00°	Depositor
Resolution (Å)	8.00 – 2.00 8.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.00) 69.2 (8.00-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.72 (at 1.90Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.200 , 0.246 0.183 , 0.224	Depositor DCC
R_{free} test set	7107 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	13.1	Xtriage
Anisotropy	0.670	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 64.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	17070	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% of the height of the origin peak. No significant pseudotranslation is detected.*

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: EPG, CA

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	0.45	1/4234 (0.0%)	0.91	17/5751 (0.3%)
1	B	0.45	1/4234 (0.0%)	0.90	16/5751 (0.3%)
1	C	0.46	1/4234 (0.0%)	0.91	13/5751 (0.2%)
1	D	0.46	1/4234 (0.0%)	0.92	16/5751 (0.3%)
All	All	0.46	4/16936 (0.0%)	0.91	62/23004 (0.3%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	172	GLU	CD-OE2	7.88	1.40	1.25
1	B	172	GLU	CD-OE2	7.83	1.40	1.25
1	D	172	GLU	CD-OE2	7.62	1.39	1.25
1	C	172	GLU	CD-OE2	7.34	1.39	1.25

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	277	ASP	N-CA-C	8.72	121.57	111.11
1	B	57	LYS	N-CA-C	8.21	120.01	111.14
1	A	57	LYS	N-CA-C	8.13	119.84	110.97
1	D	57	LYS	N-CA-C	8.09	119.79	110.97
1	C	277	ASP	N-CA-C	7.87	120.62	111.02
1	D	277	ASP	N-CA-C	7.66	120.37	111.02
1	C	58	ASN	N-CA-C	7.31	121.46	112.54
1	D	505	VAL	N-CA-C	-7.25	101.84	108.95
1	A	442	ASN	N-CA-C	7.17	118.88	111.14
1	B	334	MET	N-CA-C	6.50	120.50	110.42
1	D	337	LYS	N-CA-C	-6.47	103.45	112.12
1	B	277	ASP	N-CA-C	6.45	118.85	111.11
1	D	414	LEU	N-CA-C	6.32	119.11	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	58	ASN	N-CA-C	6.15	120.52	112.89
1	C	454	TYR	N-CA-C	6.04	123.17	109.81
1	A	331	CYS	N-CA-C	5.97	119.87	112.58
1	D	442	ASN	N-CA-C	5.92	117.73	111.28
1	A	505	VAL	N-CA-C	-5.91	103.16	108.95
1	A	55	MET	N-CA-C	5.88	119.72	112.54
1	C	389	ASN	N-CA-C	5.78	119.64	112.24
1	C	57	LYS	N-CA-C	5.75	117.24	110.97
1	B	58	ASN	N-CA-C	5.73	119.99	112.89
1	D	55	MET	N-CA-C	5.72	119.52	112.54
1	D	389	ASN	N-CA-C	5.72	119.46	111.74
1	A	342	GLU	N-CA-C	5.69	117.56	111.36
1	B	414	LEU	N-CA-C	5.66	118.30	111.40
1	A	292	HIS	N-CA-C	5.66	119.90	112.89
1	C	292	HIS	N-CA-C	5.62	120.14	113.28
1	D	292	HIS	N-CA-C	5.59	119.95	113.18
1	D	276	PHE	N-CA-C	5.58	121.11	113.97
1	A	87	SER	N-CA-C	5.57	118.47	108.17
1	C	342	GLU	N-CA-C	5.56	117.42	111.36
1	A	58	ASN	N-CA-C	5.55	119.32	112.54
1	B	196	THR	N-CA-C	-5.51	102.32	110.48
1	C	189	ARG	N-CA-C	-5.48	103.30	110.53
1	B	55	MET	N-CA-C	5.47	119.22	112.54
1	C	116	LEU	N-CA-C	5.47	119.67	112.89
1	B	63	PHE	N-CA-C	5.45	117.91	110.55
1	C	87	SER	N-CA-C	5.44	118.23	108.17
1	A	389	ASN	N-CA-C	5.42	119.06	111.74
1	A	196	THR	N-CA-C	-5.42	103.24	110.55
1	D	428	ASN	N-CA-C	5.36	118.97	111.90
1	B	233	PRO	N-CA-C	-5.31	104.22	110.70
1	A	399	GLN	N-CA-C	5.29	118.52	111.75
1	A	417	VAL	N-CA-C	5.27	117.37	109.20
1	A	276	PHE	N-CA-C	5.26	120.34	113.88
1	C	55	MET	N-CA-C	5.26	118.85	112.23
1	D	87	SER	N-CA-C	5.25	117.66	108.52
1	C	63	PHE	N-CA-C	5.24	117.63	110.55
1	A	414	LEU	N-CA-C	5.23	117.78	111.40
1	B	87	SER	N-CA-C	5.22	117.82	108.17
1	D	141	GLU	N-CA-C	5.21	116.64	111.07
1	B	276	PHE	N-CA-C	5.18	120.59	113.97
1	C	442	ASN	N-CA-C	5.17	117.82	111.82
1	B	292	HIS	N-CA-C	5.16	119.63	113.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	280	PHE	N-CA-C	5.15	119.61	112.45
1	B	415	LEU	N-CA-C	5.13	120.19	113.88
1	D	399	GLN	N-CA-C	5.12	118.31	111.75
1	A	51	TRP	N-CA-C	5.10	117.61	109.96
1	B	28	TRP	N-CA-C	5.06	116.80	111.28
1	D	280	PHE	N-CA-C	5.06	119.49	112.45
1	B	399	GLN	N-CA-C	5.02	117.40	111.33

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	4119	0	3984	42	0
1	B	4119	0	3984	58	0
1	C	4119	0	3984	49	0
1	D	4119	0	3984	61	0
2	A	16	0	15	0	0
2	B	16	0	15	0	0
2	C	16	0	15	0	0
2	D	16	0	15	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	160	0	0	1	0
4	B	103	0	0	1	0
4	C	138	0	0	0	0
4	D	125	0	0	1	0
All	All	17070	0	15996	210	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (210) 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:482:LYS:HG2	1:A:496:GLN:HB3	1.68	0.74
1:B:347:LYS:HE3	1:B:384:MET:SD	2.28	0.74
1:D:2:VAL:O	1:D:5:LYS:HG2	1.90	0.71
1:B:375:GLU:HG3	4:B:801:HOH:O	1.90	0.71
1:C:372:ILE:HG23	1:C:377:GLU:HB2	1.75	0.68
1:A:373:GLY:HA2	1:A:407:LEU:HD11	1.76	0.67
1:D:201:SER:O	1:D:205:LEU:HG	1.97	0.65
1:C:482:LYS:HG2	1:C:495:TRP:HE3	1.62	0.65
1:A:119:LYS:HD2	1:A:123:GLY:HA2	1.77	0.65
1:D:118:PHE:HB2	1:D:126:ASN:HB3	1.81	0.63
1:B:482:LYS:HG2	1:B:499:GLN:HA	1.80	0.63
1:B:372:ILE:HG23	1:B:377:GLU:HB2	1.81	0.62
1:B:7:MET:HE2	1:B:419:PRO:HB3	1.81	0.62
1:B:11:TYR:HA	1:B:391:ALA:O	1.99	0.61
1:D:337:LYS:HE3	1:D:342:GLU:OE1	2.01	0.61
1:B:426:VAL:HA	1:B:514:SER:O	2.00	0.61
1:D:488:LYS:H	1:D:488:LYS:HD3	1.65	0.61
1:D:508:LYS:HD2	1:D:508:LYS:O	2.02	0.60
1:D:337:LYS:HZ2	1:D:344:SER:H	1.51	0.59
1:C:7:MET:HE2	1:C:419:PRO:HB3	1.85	0.58
1:D:20:LYS:HD3	1:D:99:CYS:HA	1.85	0.58
1:C:422:GLN:NE2	1:C:506:PRO:HG2	2.19	0.57
1:C:482:LYS:HG3	1:C:496:GLN:HB3	1.84	0.57
1:D:337:LYS:NZ	1:D:344:SER:H	2.03	0.57
1:C:321:LYS:HA	1:C:321:LYS:HE2	1.87	0.56
1:C:429:VAL:HG22	1:C:431:THR:HG23	1.86	0.56
1:B:454:TYR:N	1:B:455:PRO:HD2	2.21	0.56
1:C:104:PRO:HB2	1:C:107:VAL:HG23	1.87	0.56
1:C:482:LYS:HD2	1:C:496:GLN:O	2.06	0.56
1:B:248:MET:HE3	1:B:251:LYS:HB2	1.88	0.56
1:B:478:ASN:ND2	1:B:503:ASN:HB3	2.20	0.56
1:B:507:LEU:H	1:B:507:LEU:HD12	1.71	0.56
1:A:482:LYS:HD3	1:A:496:GLN:O	2.06	0.55
1:D:82:MET:HE2	1:D:84:PRO:HG3	1.88	0.55
1:D:103:ILE:HD11	1:D:108:TRP:CZ2	2.41	0.55
1:B:92:GLY:HA2	1:B:97:ASP:HB3	1.89	0.54
1:A:90:GLN:HG3	1:A:102:PRO:HA	1.89	0.54
1:D:6:GLY:HA3	4:D:814:HOH:O	2.07	0.54
1:B:103:ILE:HD11	1:B:108:TRP:CZ2	2.42	0.54
1:D:119:LYS:HE2	1:D:196:THR:HA	1.90	0.54
1:B:15:LEU:HD11	1:B:398:TYR:HA	1.90	0.53
1:D:133:LEU:HB3	1:D:198:PHE:HE2	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:330:THR:O	1:D:331:CYS:HB2	2.07	0.53
1:B:57:LYS:NZ	1:B:57:LYS:HB3	2.24	0.52
1:A:355:THR:O	1:A:359:GLU:HB2	2.08	0.52
1:A:454:TYR:N	1:A:455:PRO:HD2	2.24	0.52
1:C:432:THR:HG22	1:C:433:ILE:H	1.73	0.52
1:D:434:GLY:HA3	1:D:488:LYS:HG3	1.90	0.52
1:D:208:LEU:HD11	1:D:228:GLU:HB3	1.90	0.52
1:D:335:THR:HG23	1:D:380:ARG:HD3	1.90	0.52
1:C:351:GLN:HG2	1:C:384:MET:HE1	1.91	0.52
1:B:424:ILE:O	1:B:468:ARG:HA	2.09	0.52
1:D:232:LEU:HB3	1:D:233:PRO:HD2	1.92	0.52
1:B:154:LYS:HB3	1:B:155:PRO:HD3	1.92	0.52
1:B:104:PRO:HB3	1:B:106:TRP:NE1	2.25	0.52
1:A:406:SER:O	1:A:410:LYS:HG2	2.10	0.51
1:C:55:MET:O	1:C:63:PHE:HA	2.11	0.51
1:D:344:SER:C	1:D:346:PRO:HD3	2.35	0.51
1:A:422:GLN:NE2	1:A:506:PRO:HG2	2.25	0.51
1:A:55:MET:O	1:A:63:PHE:HA	2.11	0.51
1:D:104:PRO:HB2	1:D:107:VAL:HG23	1.93	0.51
1:B:118:PHE:HB2	1:B:126:ASN:HB3	1.93	0.50
1:C:487:SER:HB2	1:C:489:ASP:OD2	2.10	0.50
1:D:454:TYR:N	1:D:455:PRO:HD2	2.27	0.50
1:A:238:GLU:O	1:A:242:MET:HG3	2.12	0.50
1:B:420:VAL:HG13	1:B:475:ALA:HB2	1.92	0.50
1:D:51:TRP:CZ2	1:D:91:CYS:SG	3.05	0.50
1:D:104:PRO:HB3	1:D:106:TRP:NE1	2.27	0.50
1:B:383:GLU:O	1:B:387:ASN:HB2	2.10	0.49
1:B:201:SER:O	1:B:205:LEU:HG	2.12	0.49
1:C:27:ASN:OD1	1:C:29:GLU:HB2	2.11	0.49
1:C:347:LYS:O	1:C:351:GLN:HG3	2.13	0.49
1:A:7:MET:HE2	1:A:419:PRO:HG3	1.94	0.49
1:C:337:LYS:HE2	1:C:344:SER:HB2	1.95	0.49
1:D:238:GLU:O	1:D:242:MET:HG3	2.12	0.49
1:A:215:ASN:O	1:A:219:LYS:HG3	2.12	0.48
1:C:134:ALA:O	1:C:138:ILE:HG12	2.12	0.48
1:C:219:LYS:NZ	1:C:219:LYS:HB3	2.27	0.48
1:B:420:VAL:CG1	1:B:475:ALA:HB2	2.43	0.48
1:D:372:ILE:HG23	1:D:377:GLU:HB2	1.95	0.48
1:B:4:GLY:HA2	1:B:455:PRO:O	2.14	0.48
1:C:453:GLN:C	1:C:455:PRO:HD2	2.38	0.48
1:A:422:GLN:HE22	1:A:506:PRO:HG2	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:PHE:O	1:B:202:LYS:HG2	2.14	0.48
1:B:454:TYR:N	1:B:455:PRO:CD	2.77	0.48
1:C:502:TRP:CH2	1:C:512:HIS:HB2	2.48	0.48
1:B:31:PHE:O	1:B:35:LEU:HG	2.14	0.48
1:B:186:TYR:CE1	1:B:293:TRP:HB3	2.49	0.48
1:A:103:ILE:HD11	1:A:108:TRP:CZ2	2.49	0.48
1:B:425:VAL:HG22	1:B:468:ARG:NH1	2.29	0.48
1:C:198:PHE:O	1:C:202:LYS:HG2	2.14	0.48
1:D:115:SER:HB3	1:D:198:PHE:CD1	2.49	0.48
1:D:300:ILE:O	1:D:300:ILE:HG13	2.14	0.48
1:C:22:ILE:HB	1:C:23:PRO:HD3	1.95	0.47
1:C:406:SER:O	1:C:410:LYS:HG2	2.14	0.47
1:B:439:ILE:HG13	1:B:456:ILE:HB	1.96	0.47
1:B:429:VAL:HG13	1:B:516:TRP:CE3	2.49	0.47
1:A:118:PHE:HB2	1:A:126:ASN:HB3	1.97	0.47
1:C:397:ARG:HG2	1:C:398:TYR:N	2.30	0.47
1:D:214:LEU:HD11	1:D:227:SER:HA	1.95	0.47
1:A:454:TYR:N	1:A:455:PRO:CD	2.78	0.47
1:B:51:TRP:CZ2	1:B:91:CYS:SG	3.08	0.47
1:B:460:TYR:HB2	1:B:467:TRP:CE2	2.50	0.47
1:D:349:LEU:O	1:D:352:ASN:HB3	2.15	0.47
1:A:329:PHE:O	1:A:366:GLY:HA2	2.14	0.47
1:C:51:TRP:CZ2	1:C:91:CYS:SG	3.08	0.47
1:C:186:TYR:HD1	1:C:293:TRP:CD2	2.33	0.46
1:C:423:THR:HB	1:C:511:SER:OG	2.16	0.46
1:D:337:LYS:HB3	1:D:337:LYS:HZ3	1.79	0.46
1:B:107:VAL:O	1:B:110:GLN:HG2	2.16	0.46
1:B:482:LYS:CG	1:B:499:GLN:HA	2.45	0.46
1:C:329:PHE:O	1:C:366:GLY:HA2	2.15	0.46
1:C:421:MET:SD	1:C:470:ASN:HB3	2.55	0.46
1:B:19:LEU:HD13	1:B:397:ARG:CZ	2.45	0.46
1:D:346:PRO:O	1:D:350:VAL:HG23	2.16	0.46
1:D:399:GLN:CD	1:D:399:GLN:H	2.23	0.46
1:A:11:TYR:HA	1:A:391:ALA:O	2.16	0.46
1:C:296:ASN:OD1	1:C:343:TYR:HB3	2.16	0.46
1:D:351:GLN:HG2	1:D:384:MET:HE1	1.98	0.46
1:D:254:LEU:HD13	1:D:311:ASN:ND2	2.31	0.46
1:D:454:TYR:N	1:D:455:PRO:CD	2.78	0.46
1:A:443:ARG:HB3	1:A:445:GLU:OE1	2.16	0.45
1:C:90:GLN:HB3	1:C:128:GLU:HB2	1.98	0.45
1:A:424:ILE:O	1:A:468:ARG:HA	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:407:LEU:HD12	1:C:407:LEU:HA	1.85	0.45
1:B:31:PHE:CE2	1:B:35:LEU:HD11	2.52	0.45
1:B:300:ILE:O	1:B:300:ILE:HG13	2.17	0.45
1:A:300:ILE:HG13	1:A:300:ILE:O	2.16	0.45
1:C:162:LYS:HG2	1:C:163:ILE:N	2.30	0.45
1:D:286:ALA:HB3	1:D:320:PHE:CE2	2.52	0.45
1:D:345:MET:N	1:D:346:PRO:HD3	2.32	0.45
1:A:306:LYS:HB2	1:A:307:PRO:HD3	1.98	0.45
1:B:347:LYS:HE2	1:B:351:GLN:NE2	2.31	0.45
1:C:201:SER:O	1:C:205:LEU:HG	2.17	0.45
1:A:422:GLN:HB2	1:A:473:LEU:HD23	2.00	0.44
1:C:498:ILE:HG23	1:C:500:GLN:NE2	2.33	0.44
1:D:286:ALA:HB3	1:D:320:PHE:HE2	1.82	0.44
1:D:424:ILE:O	1:D:468:ARG:HA	2.17	0.44
1:C:2:VAL:HG22	1:C:387:ASN:O	2.17	0.44
1:B:508:LYS:HD2	1:B:508:LYS:N	2.33	0.44
1:C:429:VAL:HA	1:C:430:PRO:HD2	1.90	0.44
1:D:7:MET:HE2	1:D:419:PRO:HB3	1.98	0.44
1:C:1:ALA:HA	1:C:387:ASN:OD1	2.17	0.44
1:C:133:LEU:HD22	1:C:202:LYS:HG3	1.99	0.44
1:D:226:ILE:HG23	1:D:227:SER:H	1.82	0.44
1:C:503:ASN:HA	1:C:504:PRO:HA	1.86	0.44
1:A:104:PRO:HB2	1:A:107:VAL:HG23	2.00	0.43
1:A:292:HIS:O	1:A:344:SER:HA	2.18	0.43
1:B:336:ASP:HA	1:B:346:PRO:HD2	2.00	0.43
1:B:428:ASN:O	1:B:516:TRP:HB3	2.18	0.43
1:A:426:VAL:HA	1:A:514:SER:O	2.19	0.43
1:B:22:ILE:HB	1:B:23:PRO:HD3	2.00	0.43
1:A:16:MET:O	1:A:398:TYR:HB2	2.18	0.43
1:B:321:LYS:HE2	1:B:360:LYS:O	2.19	0.43
1:B:344:SER:C	1:B:346:PRO:HD3	2.44	0.43
1:C:118:PHE:HB2	1:C:126:ASN:HB3	2.01	0.43
1:B:331:CYS:SG	1:B:334:MET:CE	3.06	0.43
1:D:84:PRO:HD2	1:D:162:LYS:O	2.19	0.43
1:A:429:VAL:HG12	1:A:431:THR:HG23	2.00	0.42
1:D:133:LEU:HD22	1:D:202:LYS:HD3	2.00	0.42
1:A:51:TRP:CZ2	1:A:91:CYS:SG	3.12	0.42
1:A:503:ASN:HA	1:A:504:PRO:HA	1.79	0.42
1:B:16:MET:O	1:B:398:TYR:HB2	2.19	0.42
1:C:104:PRO:HB3	1:C:106:TRP:NE1	2.35	0.42
1:D:214:LEU:HD11	1:D:227:SER:CA	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:LEU:HD21	1:A:137:VAL:HG21	2.01	0.42
1:A:336:ASP:HA	1:A:346:PRO:HD2	2.00	0.42
1:B:157:LYS:HE3	1:B:157:LYS:HB2	1.90	0.42
1:B:485:ILE:HG13	1:B:516:TRP:CH2	2.54	0.42
1:A:330:THR:O	1:A:331:CYS:HB2	2.19	0.42
1:C:202:LYS:HA	1:C:202:LYS:HD2	1.89	0.42
1:D:2:VAL:O	1:D:3:ASN:HB2	2.19	0.42
1:D:453:GLN:C	1:D:455:PRO:HD2	2.45	0.42
1:D:347:LYS:O	1:D:351:GLN:HG3	2.20	0.42
1:C:424:ILE:O	1:C:468:ARG:HA	2.20	0.42
1:D:198:PHE:O	1:D:202:LYS:HG3	2.20	0.42
1:A:317:LEU:HD12	1:A:356:LEU:HB3	2.01	0.42
1:B:85:ILE:HG12	1:B:164:TYR:HB2	2.01	0.42
1:C:399:GLN:H	1:C:399:GLN:CD	2.28	0.42
1:C:454:TYR:N	1:C:455:PRO:HD2	2.35	0.42
1:D:482:LYS:HG3	1:D:499:GLN:HA	2.01	0.41
1:A:134:ALA:O	1:A:138:ILE:HG12	2.19	0.41
1:A:354:ALA:HA	1:A:364:LEU:HD22	2.02	0.41
1:B:1:ALA:HA	1:B:387:ASN:OD1	2.20	0.41
1:B:427:LYS:HE3	1:B:427:LYS:HB3	1.84	0.41
1:B:498:ILE:HG23	1:B:500:GLN:NE2	2.35	0.41
1:D:213:SER:O	1:D:217:VAL:HG23	2.20	0.41
1:B:116:LEU:HD21	1:B:137:VAL:HG21	2.03	0.41
1:C:383:GLU:O	1:C:387:ASN:HB2	2.20	0.41
1:A:94:ASN:HB3	4:A:836:HOH:O	2.21	0.41
1:D:16:MET:HG3	1:D:394:THR:HG22	2.03	0.41
1:D:117:TYR:HB3	1:D:127:LYS:HG2	2.02	0.41
1:D:337:LYS:HE2	1:D:339:SER:OG	2.20	0.41
1:D:488:LYS:HE2	1:D:488:LYS:HB2	1.91	0.41
1:B:225:LEU:HD22	1:B:230:ALA:HB1	2.03	0.41
1:D:337:LYS:NZ	1:D:337:LYS:HB3	2.35	0.41
1:A:84:PRO:HD2	1:A:162:LYS:O	2.20	0.41
1:B:186:TYR:HD1	1:B:293:TRP:CD2	2.39	0.41
1:B:461:ASP:HB3	1:B:464:SER:OG	2.19	0.41
1:C:16:MET:HG3	1:C:394:THR:HG22	2.03	0.41
1:D:406:SER:O	1:D:410:LYS:HG2	2.21	0.41
1:A:423:THR:HB	1:A:511:SER:HB3	2.03	0.41
1:B:425:VAL:HG22	1:B:468:ARG:HH12	1.86	0.41
1:D:421:MET:SD	1:D:470:ASN:HB3	2.61	0.40
1:A:157:LYS:HE3	1:A:157:LYS:HB2	1.92	0.40
1:D:337:LYS:HZ1	1:D:343:TYR:H	1.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:37:TRP:O	1:D:40:GLN:HB2	2.22	0.40
1:A:429:VAL:HA	1:A:430:PRO:HD3	1.86	0.40
1:C:397:ARG:HG2	1:C:398:TYR:H	1.86	0.40
1:D:503:ASN:HA	1:D:504:PRO:HA	1.80	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	514/516 (100%)	488 (95%)	25 (5%)	1 (0%)	43	42
1	B	514/516 (100%)	492 (96%)	20 (4%)	2 (0%)	30	27
1	C	514/516 (100%)	490 (95%)	23 (4%)	1 (0%)	43	42
1	D	514/516 (100%)	492 (96%)	20 (4%)	2 (0%)	30	27
All	All	2056/2064 (100%)	1962 (95%)	88 (4%)	6 (0%)	36	35

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	398	TYR
1	C	398	TYR
1	D	398	TYR
1	B	398	TYR
1	D	26	THR
1	B	428	ASN

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	440/440 (100%)	433 (98%)	7 (2%)	55	62
1	B	440/440 (100%)	427 (97%)	13 (3%)	36	38
1	C	440/440 (100%)	422 (96%)	18 (4%)	27	26
1	D	440/440 (100%)	424 (96%)	16 (4%)	31	31
All	All	1760/1760 (100%)	1706 (97%)	54 (3%)	35	37

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	LEU
1	A	299	THR
1	A	349	LEU
1	A	356	LEU
1	A	377	GLU
1	A	482	LYS
1	A	507	LEU
1	B	19	LEU
1	B	57	LYS
1	B	109	ASN
1	B	279	THR
1	B	332	LEU
1	B	349	LEU
1	B	423	THR
1	B	427	LYS
1	B	436	THR
1	B	453	GLN
1	B	473	LEU
1	B	488	LYS
1	B	504	PRO
1	C	19	LEU
1	C	187	PRO
1	C	219	LYS
1	C	279	THR
1	C	300	ILE
1	C	321	LYS
1	C	335	THR
1	C	349	LEU

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Mol	Chain	Res	Type
1	C	377	GLU
1	C	380	ARG
1	C	399	GLN
1	C	429	VAL
1	C	432	THR
1	C	436	THR
1	C	462	SER
1	C	464	SER
1	C	502	TRP
1	C	504	PRO
1	D	112	SER
1	D	158	ASP
1	D	187	PRO
1	D	202	LYS
1	D	214	LEU
1	D	228	GLU
1	D	305	GLU
1	D	337	LYS
1	D	349	LEU
1	D	399	GLN
1	D	433	ILE
1	D	452	LYS
1	D	473	LEU
1	D	504	PRO
1	D	508	LYS
1	D	510	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	ASN
1	A	215	ASN
1	A	292	HIS
1	A	351	GLN
1	A	428	ASN
1	A	453	GLN
1	A	478	ASN
1	B	58	ASN
1	B	292	HIS
1	B	311	ASN
1	B	351	GLN
1	B	389	ASN

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Mol	Chain	Res	Type
1	B	405	ASN
1	B	428	ASN
1	B	453	GLN
1	B	463	HIS
1	B	478	ASN
1	B	500	GLN
1	B	503	ASN
1	C	40	GLN
1	C	73	GLN
1	C	352	ASN
1	C	470	ASN
1	C	500	GLN
1	D	3	ASN
1	D	62	GLN
1	D	239	GLN
1	D	281	GLN
1	D	292	HIS
1	D	302	HIS
1	D	311	ASN
1	D	428	ASN
1	D	463	HIS
1	D	478	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](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	EPG	B	601	1	17,17,17	5.46	2 (11%)	24,24,24	5.03	5 (20%)
2	EPG	D	601	1	17,17,17	5.42	2 (11%)	24,24,24	5.00	5 (20%)
2	EPG	A	601	1	17,17,17	5.39	2 (11%)	24,24,24	4.99	5 (20%)
2	EPG	C	601	1	17,17,17	5.64	2 (11%)	24,24,24	4.97	6 (25%)

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	EPG	B	601	1	-	1/7/29/29	0/2/2/2
2	EPG	D	601	1	-	1/7/29/29	0/2/2/2
2	EPG	A	601	1	-	1/7/29/29	0/2/2/2
2	EPG	C	601	1	-	2/7/29/29	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	EPG	O8-C9	22.74	2.46	1.43
2	B	601	EPG	O8-C9	22.25	2.43	1.43
2	D	601	EPG	O8-C9	22.11	2.43	1.43
2	A	601	EPG	O8-C9	22.03	2.42	1.43
2	C	601	EPG	C9-C8	3.25	1.56	1.44
2	D	601	EPG	C9-C8	2.16	1.52	1.44
2	B	601	EPG	C9-C8	2.09	1.52	1.44
2	A	601	EPG	C9-C8	2.01	1.51	1.44

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	EPG	O8-C8-C9	19.96	110.63	59.95
2	D	601	EPG	O8-C8-C9	19.85	110.36	59.95
2	A	601	EPG	O8-C8-C9	19.85	110.35	59.95
2	C	601	EPG	O8-C8-C9	19.59	109.70	59.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	EPG	O8-C9-C8	-9.97	33.53	59.66
2	B	601	EPG	O8-C9-C8	-9.91	33.68	59.66
2	D	601	EPG	O8-C9-C8	-9.90	33.70	59.66
2	A	601	EPG	O8-C9-C8	-9.87	33.79	59.66
2	B	601	EPG	C9-O8-C8	-8.63	35.69	60.40
2	A	601	EPG	C9-O8-C8	-8.58	35.85	60.40
2	D	601	EPG	C9-O8-C8	-8.54	35.95	60.40
2	C	601	EPG	C9-O8-C8	-8.26	36.77	60.40
2	B	601	EPG	O1-C1-C2	4.56	115.20	108.27
2	C	601	EPG	O1-C1-C2	4.51	115.13	108.27
2	A	601	EPG	O1-C1-C2	4.34	114.87	108.27
2	D	601	EPG	O1-C1-C2	4.30	114.81	108.27
2	C	601	EPG	C7-C8-C9	-2.56	107.40	120.60
2	A	601	EPG	C7-C8-C9	-2.44	108.00	120.60
2	D	601	EPG	C7-C8-C9	-2.36	108.44	120.60
2	B	601	EPG	C7-C8-C9	-2.35	108.47	120.60
2	C	601	EPG	C1-C2-C3	-2.23	105.32	110.01

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	EPG	O1-C7-C8-C9
2	B	601	EPG	O1-C7-C8-C9
2	D	601	EPG	O1-C7-C8-C9
2	C	601	EPG	O1-C7-C8-C9
2	C	601	EPG	C4-C5-C6-O6

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	516/516 (100%)	-0.73	1 (0%) 91 90	2, 12, 33, 53	0
1	B	516/516 (100%)	-0.49	6 (1%) 76 76	3, 16, 42, 61	0
1	C	516/516 (100%)	-0.64	2 (0%) 88 88	3, 15, 38, 56	0
1	D	516/516 (100%)	-0.56	1 (0%) 91 90	3, 15, 38, 48	0
All	All	2064/2064 (100%)	-0.61	10 (0%) 87 87	2, 15, 39, 61	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	433	ILE	3.9
1	B	489	ASP	2.8
1	B	433	ILE	2.6
1	B	431	THR	2.6
1	B	463	HIS	2.5
1	B	462	SER	2.4
1	C	487	SER	2.2
1	C	463	HIS	2.1
1	D	1	ALA	2.1
1	B	215	ASN	2.1

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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
2	EPG	B	601	16/16	0.92	0.07	9,16,28,28	0
3	CA	B	701	1/1	0.92	0.01	3,3,3,3	0
2	EPG	C	601	16/16	0.93	0.06	7,12,25,26	0
2	EPG	A	601	16/16	0.93	0.06	4,12,21,22	0
2	EPG	D	601	16/16	0.95	0.05	9,13,23,24	0
3	CA	D	701	1/1	0.97	0.03	12,12,12,12	0
3	CA	C	701	1/1	0.99	0.05	6,6,6,6	0
3	CA	A	701	1/1	1.00	0.02	7,7,7,7	0

6.5 Other polymers [i](#)

There are no such residues in this entry.