Full wwPDB X-ray Structure Validation Report (i)

May 23, 2020 – 06:11 pm BST

PDB ID	:	5F0K
Title	:	Structure of VPS35 N terminal region
Authors	:	Lucas, M.; Gershlick, D.; Vidaurrazaga, A.; Rojas, A.L.; Bonifacino, J.S.; Hierro, A.
Deposited on	:	2015-11-27
Resolution	:	3.07 Å(reported)

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

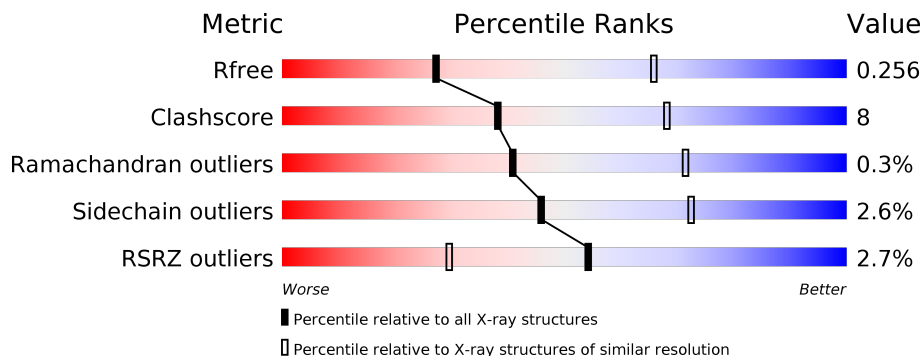|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 3.07 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

Metric	Percentile Ranks	Value
Rfree		0.256
Clashscore		8
Ramachandran outliers		0.3%
Sidechain outliers		2.6%
RSRZ outliers		2.7%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	1447 (3.10-3.06)
Clashscore	141614	1546 (3.10-3.06)
Ramachandran outliers	138981	1487 (3.10-3.06)
Sidechain outliers	138945	1486 (3.10-3.06)
RSRZ outliers	127900	1416 (3.10-3.06)

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 on 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	462	2%　79%　15%　6%
1	B	462	2%　71%　20%　· 7%
1	C	462	4%　74%　19%　· 5%
1	D	462	2%　82%　11%　· 6%
1	E	462	3%　73%　17%　· 8%

2   Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 35602 atoms, of which 17991 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 Vacuolar protein sorting-associated protein 35.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	433	Total 7075	C 2237	H 3571	N 592	O 653	S 22	0	0	0
1	B	430	Total 7043	C 2225	H 3559	N 587	O 649	S 23	0	0	0
1	C	439	Total 7159	C 2253	H 3618	N 604	O 661	S 23	0	0	0
1	D	433	Total 7080	C 2238	H 3577	N 591	O 651	S 23	0	0	0
1	E	423	Total 6915	C 2180	H 3492	N 583	O 638	S 22	0	0	0

There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	GLY	-	expression tag	UNP Q96QK1
A	10	ALA	-	expression tag	UNP Q96QK1
A	11	MET	-	expression tag	UNP Q96QK1
A	12	GLY	-	expression tag	UNP Q96QK1
A	13	SER	-	expression tag	UNP Q96QK1
B	9	GLY	-	expression tag	UNP Q96QK1
B	10	ALA	-	expression tag	UNP Q96QK1
B	11	MET	-	expression tag	UNP Q96QK1
B	12	GLY	-	expression tag	UNP Q96QK1
B	13	SER	-	expression tag	UNP Q96QK1
C	9	GLY	-	expression tag	UNP Q96QK1
C	10	ALA	-	expression tag	UNP Q96QK1
C	11	MET	-	expression tag	UNP Q96QK1
C	12	GLY	-	expression tag	UNP Q96QK1
C	13	SER	-	expression tag	UNP Q96QK1
D	9	GLY	-	expression tag	UNP Q96QK1
D	10	ALA	-	expression tag	UNP Q96QK1
D	11	MET	-	expression tag	UNP Q96QK1
D	12	GLY	-	expression tag	UNP Q96QK1

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Chain	Residue	Modelled	Actual	Comment	Reference
D	13	SER	-	expression tag	UNP Q96QK1
E	9	GLY	-	expression tag	UNP Q96QK1
E	10	ALA	-	expression tag	UNP Q96QK1
E	11	MET	-	expression tag	UNP Q96QK1
E	12	GLY	-	expression tag	UNP Q96QK1
E	13	SER	-	expression tag	UNP Q96QK1

• 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 10	C 2	H 6	O 2	0	0
2	A	1	Total 10	C 2	H 6	O 2	0	0
2	A	1	Total 10	C 2	H 6	O 2	0	0
2	A	1	Total 10	C 2	H 6	O 2	0	0
2	A	1	Total 10	C 2	H 6	O 2	0	0
2	B	1	Total 10	C 2	H 6	O 2	0	0
2	B	1	Total 10	C 2	H 6	O 2	0	0
2	C	1	Total 10	C 2	H 6	O 2	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total 10	C 2	H 6	O 2	0	0
2	D	1	Total 10	C 2	H 6	O 2	0	0
2	D	1	Total 10	C 2	H 6	O 2	0	0
2	D	1	Total 10	C 2	H 6	O 2	0	0
2	E	1	Total 10	C 2	H 6	O 2	0	0
2	E	1	Total 10	C 2	H 6	O 2	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
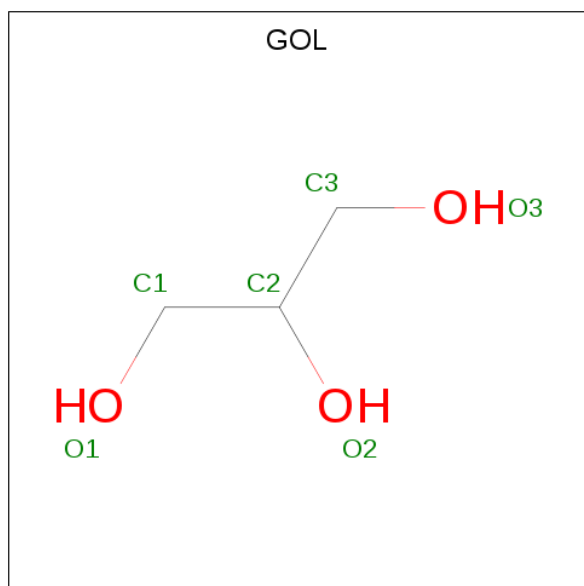
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 14	C 3	H 8	O 3	0	0
3	B	1	Total 14	C 3	H 8	O 3	0	0
3	B	1	Total 14	C 3	H 8	O 3	0	0
3	B	1	Total 14	C 3	H 8	O 3	0	0
3	C	1	Total 14	C 3	H 8	O 3	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	D	1	Total	C	H	O	0	0
			14	3	8	3		
3	D	1	Total	C	H	O	0	0
			14	3	8	3		
3	E	1	Total	C	H	O	0	0
			14	3	8	3		
3	E	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
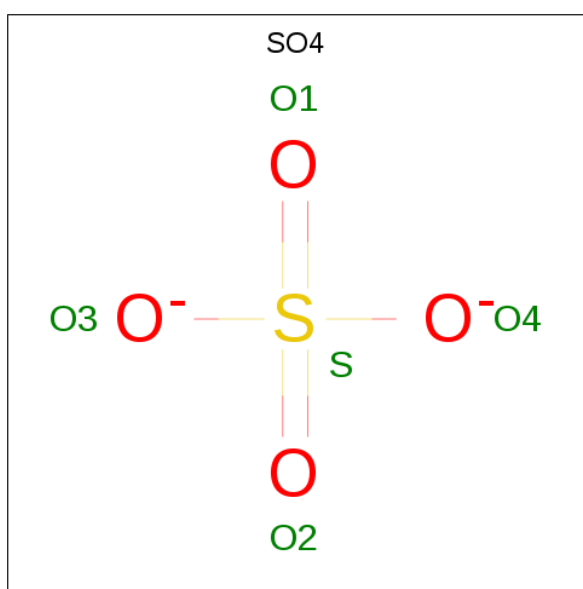
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).

PG4
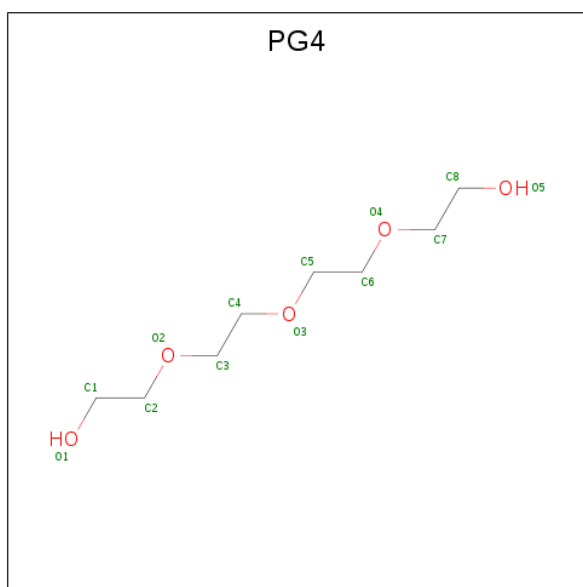
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total 31	C 8	H 18	O 5	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	7	Total 7	O 7	0	0
6	B	7	Total 7	O 7	0	0
6	E	4	Total 4	O 4	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view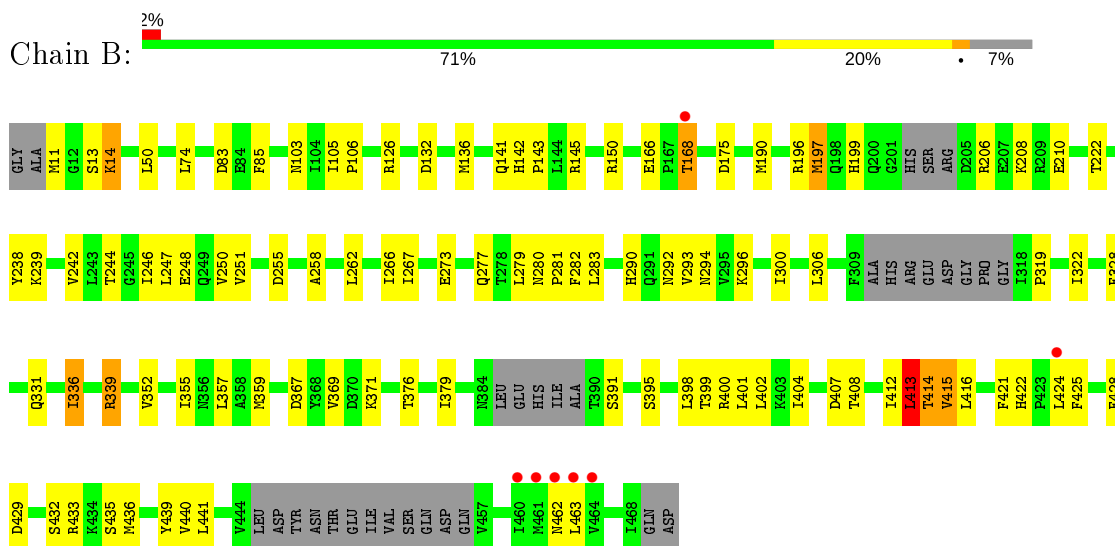 annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (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.
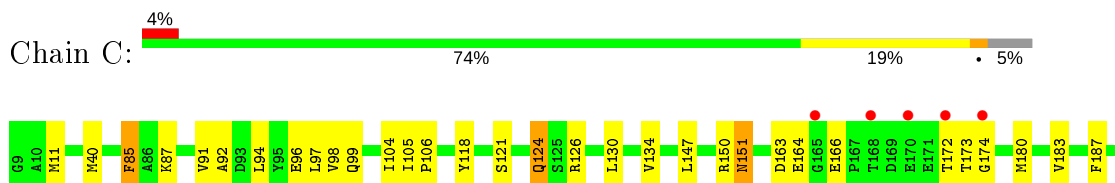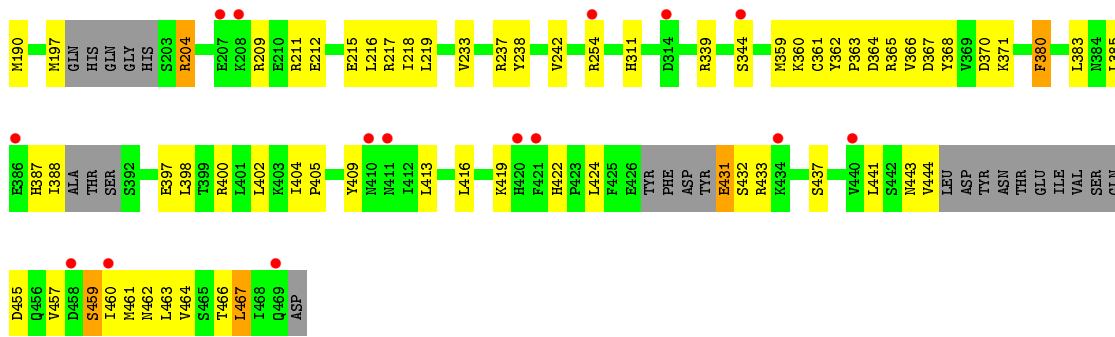
- Molecule 1: Vacuolar protein sorting-associated protein 35
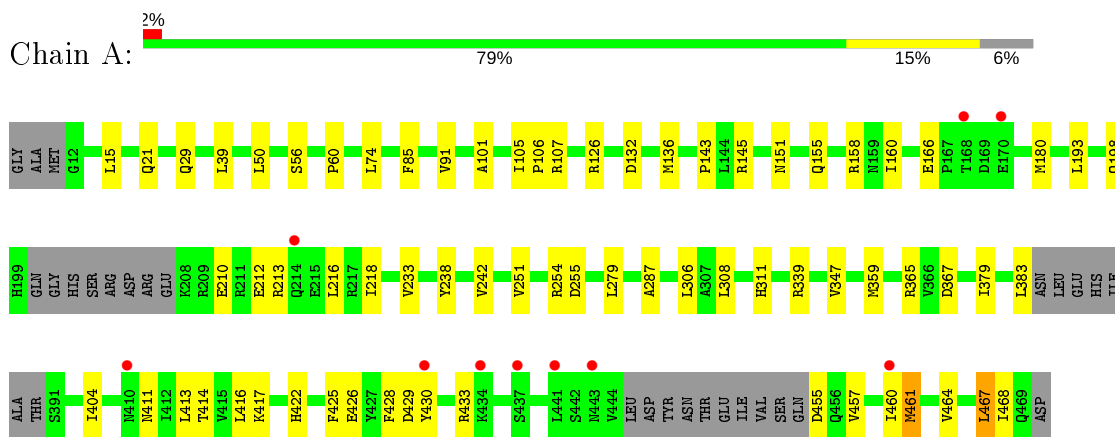
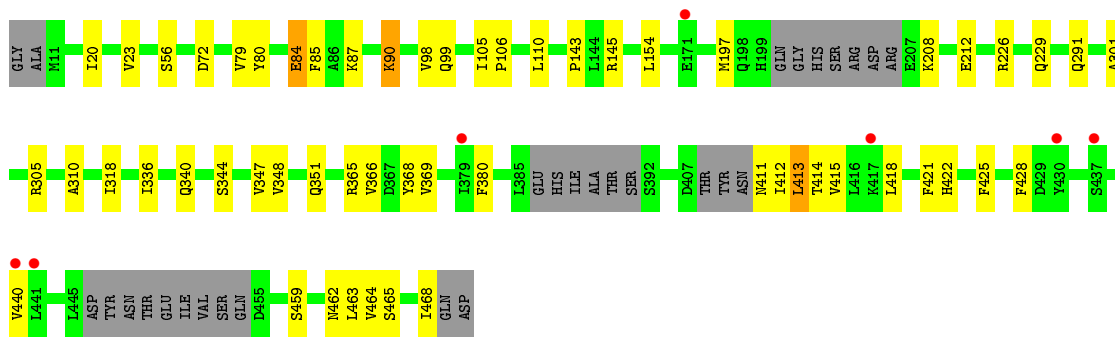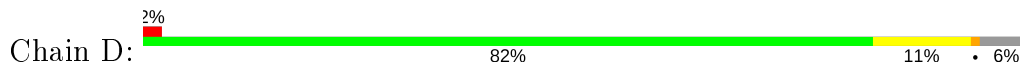- Molecule 1: Vacuolar protein sorting-associated protein 35

- Molecule 1: Vacuolar protein sorting-associated protein 35

• Molecule 1: Vacuolar protein sorting-associated protein 35

Chain D:

• Molecule 1: Vacuolar protein sorting-associated protein 35

Chain E:
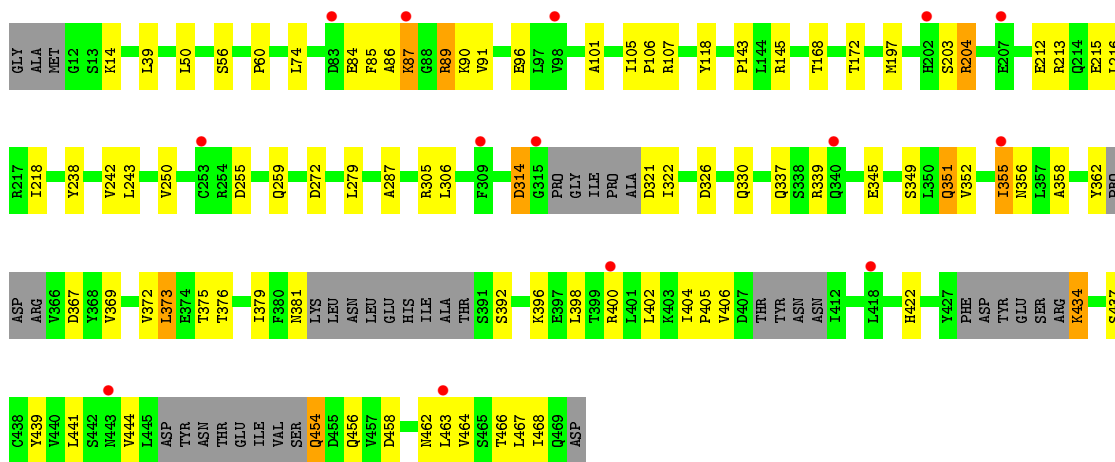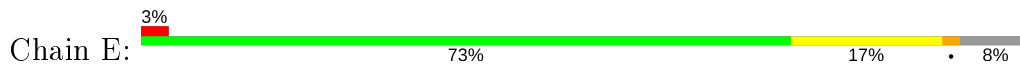
4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	200.70Å 108.60Å 167.90Å 90.00° 125.50° 90.00°	Depositor
Resolution (Å)	47.91 – 3.07	Depositor
	47.91 – 3.07	EDS
% Data completeness	99.5 (47.91-3.07)	Depositor
(in resolution range)	99.5 (47.91-3.07)	EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.82 (at 3.07Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.206 , 0.255	Depositor
	0.207 , 0.256	DCC
R_{free} test set	2725 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	53.9	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 61.4	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.002 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	35602	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.80% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: GOL, PG4, SO4, 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	0.25	0/3559	0.41	0/4808
1	B	0.26	0/3536	0.45	1/4774 (0.0%)
1	C	0.27	0/3592	0.46	1/4848 (0.0%)
1	D	0.25	0/3556	0.42	0/4801
1	E	0.27	0/3470	0.44	0/4678
All	All	0.26	0/17713	0.44	2/23909 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	413	LEU	CA-CB-CG	5.19	127.25	115.30
1	C	461	MET	CG-SD-CE	-5.15	91.96	100.20

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	3504	3571	3571	46	0
1	B	3484	3559	3558	64	0
1	C	3541	3618	3618	64	0
1	D	3503	3577	3578	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	3423	3492	3491	67	0
2	A	20	30	30	0	0
2	B	8	12	12	0	0
2	C	8	12	12	0	0
2	D	12	18	18	0	0
2	E	8	12	12	0	0
3	A	6	8	8	0	0
3	B	18	24	24	0	0
3	C	6	8	8	0	0
3	D	12	16	16	0	0
3	E	12	16	16	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	E	5	0	0	0	0
5	C	13	18	18	0	0
6	A	7	0	0	0	0
6	B	7	0	0	0	0
6	E	4	0	0	0	0
All	All	17611	17991	17990	269	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 8.

All (269) 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:21:GLN:NE2	1:D:72:ASP:OD1	2.08	0.86
1:B:141:GLN:O	1:B:196:ARG:NH2	2.10	0.84
1:C:364:ASP:O	1:C:366:VAL:N	2.21	0.74
1:C:457:VAL:HA	1:C:460:ILE:HD12	1.70	0.74
1:E:314:ASP:OD2	1:E:314:ASP:N	2.20	0.73
1:A:151:ASN:OD1	1:B:14:LYS:NZ	2.21	0.73
1:E:85:PHE:HE1	1:E:91:VAL:HG22	1.53	0.73
1:E:381:ASN:ND2	1:E:381:ASN:O	2.24	0.71
1:E:84:GLU:OE1	1:E:85:PHE:N	2.25	0.70
1:A:198:GLN:NE2	1:A:210:GLU:OE2	2.28	0.66
1:C:126:ARG:NH1	1:C:166:GLU:OE2	2.28	0.65
1:C:416:LEU:HD23	1:C:416:LEU:N	2.12	0.63
1:E:441:LEU:HD11	1:E:467:LEU:HD13	1.80	0.63
1:E:434:LYS:O	1:E:437:SER:OG	2.13	0.62
1:C:443:ASN:OD1	1:C:444:VAL:N	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:267:ILE:HD11	1:B:282:PHE:CZ	2.35	0.61
1:B:126:ARG:NH1	1:B:166:GLU:OE1	2.30	0.61
1:C:212:GLU:OE1	1:C:212:GLU:N	2.34	0.61
1:C:416:LEU:HD22	1:C:460:ILE:CD1	2.31	0.61
1:C:416:LEU:HD22	1:C:460:ILE:HD11	1.83	0.60
1:C:363:PRO:O	1:C:409:TYR:OH	2.18	0.60
1:C:370:ASP:OD1	1:C:419:LYS:N	2.34	0.60
1:E:464:VAL:HA	1:E:467:LEU:HD12	1.83	0.60
1:E:84:GLU:OE1	1:E:85:PHE:CD2	2.55	0.60
1:A:429:ASP:OD1	1:A:430:TYR:N	2.34	0.59
1:D:412:ILE:O	1:D:415:VAL:HG13	2.02	0.59
1:C:209:ARG:HG2	1:C:209:ARG:O	2.02	0.59
1:E:279:LEU:HD11	1:E:306:LEU:HD11	1.84	0.59
1:C:441:LEU:CD2	1:C:464:VAL:HG11	2.33	0.58
1:E:351:GLN:HG3	1:E:372:VAL:CG1	2.33	0.58
1:E:422:HIS:CE1	1:E:466:THR:HG21	2.39	0.58
1:C:183:VAL:O	1:C:187:PHE:N	2.33	0.57
1:E:250:VAL:O	1:E:259:GLN:NE2	2.37	0.57
1:C:460:ILE:HA	1:C:463:LEU:HD12	1.86	0.57
1:A:411:ASN:O	1:A:414:THR:OG1	2.17	0.56
1:A:213:ARG:NH2	1:A:255:ASP:OD2	2.30	0.56
1:C:431:GLU:OE1	1:C:432:SER:N	2.38	0.56
1:C:87:LYS:HA	1:C:121:SER:HB2	1.87	0.56
1:C:173:THR:HG22	1:C:174:GLY:H	1.71	0.55
1:E:355:ILE:HG13	1:E:356:ASN:N	2.21	0.55
1:A:359:MET:HE1	1:A:404:ILE:HG22	1.88	0.55
1:E:349:SER:O	1:E:352:VAL:HG12	2.07	0.55
1:C:441:LEU:HD21	1:C:464:VAL:HG11	1.88	0.55
1:C:92:ALA:O	1:C:96:GLU:HG2	2.07	0.55
1:E:462:ASN:O	1:E:466:THR:HG23	2.07	0.54
1:B:398:LEU:HD11	1:B:424:LEU:HD11	1.88	0.54
1:E:463:LEU:O	1:E:467:LEU:HG	2.07	0.54
1:C:455:ASP:OD1	1:C:455:ASP:N	2.41	0.53
1:B:415:VAL:O	1:B:415:VAL:HG13	2.08	0.53
1:E:89:ARG:O	1:E:90:LYS:HB2	2.08	0.53
1:B:279:LEU:HD21	1:B:306:LEU:HD11	1.89	0.53
1:D:226:ARG:NH2	1:D:229:GLN:OE1	2.33	0.53
1:E:441:LEU:CD1	1:E:467:LEU:HD13	2.38	0.53
1:D:336:ILE:HD13	1:D:347:VAL:HG23	1.91	0.53
1:C:422:HIS:NE2	1:C:467:LEU:HD21	2.23	0.53
1:E:326:ASP:O	1:E:330:GLN:HG2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:355:ILE:HG22	1:E:372:VAL:HB	1.89	0.53
1:C:124:GLN:OE1	1:C:172:THR:OG1	2.27	0.53
1:B:290:HIS:O	1:B:339:ARG:NH2	2.42	0.53
1:A:426:GLU:O	1:A:433:ARG:NH2	2.42	0.52
1:B:391:SER:N	1:B:429:ASP:OD1	2.43	0.52
1:E:85:PHE:CE1	1:E:91:VAL:HG22	2.39	0.52
1:D:412:ILE:HB	1:D:415:VAL:HG22	1.92	0.52
1:C:204:ARG:HD2	1:C:204:ARG:H	1.74	0.52
1:E:203:SER:O	1:E:204:ARG:HG2	2.10	0.52
1:A:50:LEU:HD21	1:A:74:LEU:HD11	1.92	0.52
1:B:283:LEU:HB3	1:B:331:GLN:HG2	1.91	0.52
1:A:428:PHE:HB2	1:A:433:ARG:HG2	1.92	0.51
1:B:238:TYR:HA	1:B:242:VAL:HG22	1.91	0.51
1:B:206:ARG:NE	1:B:210:GLU:OE2	2.43	0.51
1:C:215:GLU:N	1:C:215:GLU:OE1	2.42	0.51
1:D:85:PHE:CE1	1:D:90:LYS:HD3	2.45	0.51
1:A:101:ALA:O	1:A:107:ARG:NH1	2.43	0.51
1:E:367:ASP:N	1:E:367:ASP:OD1	2.44	0.51
1:A:218:ILE:HG21	1:B:11:MET:N	2.27	0.50
1:D:366:VAL:O	1:D:369:VAL:HG12	2.11	0.50
1:D:412:ILE:HD12	1:D:414:THR:N	2.26	0.50
1:C:11:MET:HB2	1:E:218:ILE:HD12	1.94	0.50
1:B:402:LEU:HD21	1:B:424:LEU:HD12	1.93	0.50
1:C:339:ARG:N	1:C:339:ARG:HD2	2.27	0.50
1:E:91:VAL:HG11	1:E:118:TYR:HA	1.93	0.50
1:A:367:ASP:N	1:A:367:ASP:OD1	2.45	0.50
1:D:347:VAL:O	1:D:351:GLN:HG2	2.10	0.50
1:C:367:ASP:OD1	1:C:367:ASP:N	2.44	0.50
1:C:464:VAL:HA	1:C:467:LEU:HG	1.94	0.50
1:D:105:ILE:HB	1:D:106:PRO:HD3	1.94	0.50
1:E:355:ILE:CD1	1:E:404:ILE:HD11	2.42	0.50
1:B:428:PHE:HB2	1:B:433:ARG:HB2	1.93	0.49
1:B:395:SER:O	1:B:399:THR:HG23	2.13	0.49
1:C:85:PHE:CE2	1:C:91:VAL:HG22	2.47	0.49
1:B:11:MET:HB3	1:B:13:SER:OG	2.12	0.49
1:B:413:LEU:O	1:B:415:VAL:N	2.45	0.49
1:D:208:LYS:O	1:D:212:GLU:N	2.44	0.49
1:B:246:ILE:O	1:B:250:VAL:HG23	2.11	0.49
1:B:290:HIS:O	1:B:293:VAL:HG12	2.13	0.49
1:A:105:ILE:HB	1:A:106:PRO:HD3	1.94	0.49
1:A:347:VAL:HG11	1:A:379:ILE:HG21	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:197:MET:SD	1:C:216:LEU:HD12	2.52	0.49
1:C:397:GLU:N	1:C:397:GLU:OE1	2.46	0.49
1:A:56:SER:OG	1:A:145:ARG:NH2	2.42	0.48
1:D:98:VAL:HG21	1:D:110:LEU:HB3	1.95	0.48
1:C:368:TYR:O	1:C:371:LYS:N	2.46	0.48
1:B:50:LEU:HD21	1:B:74:LEU:HD11	1.94	0.48
1:E:105:ILE:HB	1:E:106:PRO:HD3	1.95	0.48
1:B:273:GLU:N	1:B:273:GLU:OE1	2.42	0.48
1:D:418:LEU:HB3	1:D:421:PHE:HB2	1.96	0.48
1:A:455:ASP:OD1	1:A:457:VAL:HG12	2.13	0.48
1:C:180:MET:HE3	1:C:237:ARG:HD3	1.95	0.48
1:D:414:THR:HG23	1:D:414:THR:O	2.13	0.48
1:E:56:SER:HB3	1:E:145:ARG:HH12	1.79	0.48
1:E:345:GLU:OE1	1:E:392:SER:OG	2.28	0.48
1:A:39:LEU:HD13	1:A:85:PHE:HZ	1.79	0.48
1:E:101:ALA:O	1:E:107:ARG:NH1	2.44	0.47
1:E:86:ALA:O	1:E:87:LYS:HB2	2.13	0.47
1:E:358:ALA:O	1:E:362:TYR:N	2.43	0.47
1:E:422:HIS:NE2	1:E:466:THR:HG21	2.29	0.47
1:D:412:ILE:O	1:D:415:VAL:N	2.48	0.47
1:E:454:GLN:NE2	1:E:458:ASP:OD1	2.45	0.47
1:A:457:VAL:O	1:A:460:ILE:HG13	2.14	0.47
1:E:321:ASP:OD2	1:E:322:ILE:N	2.42	0.47
1:B:222:THR:HG21	1:E:14:LYS:HE3	1.96	0.47
1:E:376:THR:CB	1:E:400:ARG:HH22	2.27	0.47
1:A:29:GLN:HG3	1:D:79:VAL:CG1	2.45	0.47
1:E:464:VAL:HG22	1:E:467:LEU:HD12	1.97	0.47
1:C:40:MET:SD	1:C:97:LEU:HD22	2.55	0.47
1:D:344:SER:HA	1:D:347:VAL:HG12	1.97	0.47
1:B:293:VAL:HG12	1:B:339:ARG:HH21	1.80	0.47
1:C:383:LEU:HD23	1:C:385:LEU:H	1.80	0.47
1:D:301:ALA:O	1:D:305:ARG:HG2	2.15	0.47
1:A:422:HIS:HA	1:A:425:PHE:HD1	1.80	0.46
1:B:412:ILE:CG2	1:B:414:THR:OG1	2.63	0.46
1:B:132:ASP:O	1:B:136:MET:HG3	2.15	0.46
1:C:398:LEU:HD13	1:C:402:LEU:HD23	1.97	0.46
1:A:287:ALA:O	1:A:339:ARG:NH1	2.49	0.46
1:B:414:THR:HB	1:B:416:LEU:HD13	1.97	0.46
1:B:328:PHE:HD2	1:B:357:LEU:HD22	1.81	0.46
1:A:251:VAL:O	1:A:254:ARG:NH1	2.49	0.46
1:A:379:ILE:O	1:A:383:LEU:HG	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:319:PRO:HG2	1:B:322:ILE:HD13	1.97	0.46
1:B:355:ILE:HD11	1:B:369:VAL:HG13	1.96	0.46
1:C:463:LEU:O	1:C:466:THR:OG1	2.32	0.46
1:E:349:SER:OG	1:E:396:LYS:HE2	2.16	0.46
1:A:433:ARG:HD3	1:A:467:LEU:HD21	1.98	0.46
1:C:459:SER:O	1:C:463:LEU:HG	2.17	0.45
1:A:85:PHE:HD2	1:A:91:VAL:CG1	2.30	0.45
1:C:311:HIS:NE2	1:C:360:LYS:HB3	2.32	0.45
1:C:380:PHE:O	1:C:383:LEU:HB3	2.15	0.45
1:A:126:ARG:NH1	1:A:166:GLU:OE2	2.49	0.45
1:D:143:PRO:HB2	1:D:197:MET:HG3	1.97	0.45
1:B:244:THR:O	1:B:248:GLU:HG3	2.17	0.45
1:E:376:THR:OG1	1:E:400:ARG:NH2	2.49	0.45
1:D:412:ILE:O	1:D:413:LEU:C	2.55	0.45
1:A:308:LEU:HD12	1:B:199:HIS:HA	1.98	0.45
1:C:238:TYR:HA	1:C:242:VAL:HB	1.97	0.45
1:B:247:LEU:O	1:B:251:VAL:HG22	2.17	0.45
1:D:56:SER:HB3	1:D:145:ARG:HH21	1.80	0.45
1:E:50:LEU:HD21	1:E:74:LEU:HD11	1.98	0.45
1:B:402:LEU:HD22	1:B:421:PHE:CD1	2.52	0.44
1:E:143:PRO:HB3	1:E:197:MET:HG3	1.99	0.44
1:E:272:ASP:OD1	1:E:305:ARG:NE	2.51	0.44
1:C:147:LEU:HB3	1:C:219:LEU:HD23	2.00	0.44
1:E:404:ILE:HB	1:E:405:PRO:HD3	1.98	0.44
1:E:441:LEU:O	1:E:444:VAL:HG12	2.17	0.44
1:B:402:LEU:HD12	1:B:428:PHE:CZ	2.53	0.44
1:B:142:HIS:CD2	1:B:145:ARG:HH21	2.35	0.44
1:C:92:ALA:HA	1:C:118:TYR:HE1	1.83	0.44
1:B:336:ILE:HG21	1:B:379:ILE:HD11	1.99	0.44
1:C:150:ARG:HB3	1:C:190:MET:HE2	2.00	0.44
1:D:459:SER:O	1:D:463:LEU:HG	2.18	0.44
1:E:287:ALA:O	1:E:339:ARG:NH2	2.50	0.44
1:A:60:PRO:HB3	1:A:216:LEU:HD21	2.00	0.44
1:A:279:LEU:HD21	1:A:306:LEU:HD11	2.00	0.44
1:B:279:LEU:HD21	1:B:306:LEU:CD1	2.48	0.43
1:E:369:VAL:O	1:E:373:LEU:HD12	2.18	0.43
1:E:85:PHE:HB2	1:E:89:ARG:HE	1.83	0.43
1:C:462:ASN:O	1:C:466:THR:HG23	2.18	0.43
1:B:290:HIS:HD2	1:B:292:ASN:H	1.66	0.43
1:B:367:ASP:N	1:B:367:ASP:OD1	2.45	0.43
1:C:437:SER:OG	1:C:467:LEU:HD12	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:355:ILE:HG22	1:E:372:VAL:CB	2.47	0.43
1:B:143:PRO:HB2	1:B:197:MET:HG3	2.01	0.43
1:B:280:ASN:HB2	1:B:281:PRO:HD3	2.00	0.43
1:B:441:LEU:HD21	1:B:463:LEU:HB3	1.99	0.43
1:C:387:HIS:O	1:C:388:ILE:C	2.57	0.43
1:C:416:LEU:HD22	1:C:460:ILE:HD13	2.01	0.43
1:A:180:MET:HE3	1:A:233:VAL:HG22	2.01	0.43
1:D:412:ILE:HD12	1:D:414:THR:CA	2.48	0.43
1:D:440:VAL:CG2	1:D:463:LEU:HD13	2.48	0.43
1:A:311:HIS:O	1:B:199:HIS:ND1	2.52	0.43
1:B:422:HIS:CE1	1:B:462:ASN:HB3	2.53	0.43
1:C:209:ARG:C	1:C:211:ARG:N	2.72	0.43
1:D:462:ASN:O	1:D:465:SER:OG	2.29	0.43
1:E:39:LEU:CD1	1:E:85:PHE:HE2	2.31	0.43
1:E:86:ALA:O	1:E:89:ARG:HG2	2.19	0.43
1:A:414:THR:HA	1:A:417:LYS:HD2	2.01	0.43
1:D:80:TYR:O	1:D:84:GLU:HB2	2.19	0.43
1:E:402:LEU:O	1:E:406:VAL:HG12	2.19	0.43
1:A:155:GLN:O	1:A:158:ARG:NH1	2.52	0.42
1:B:132:ASP:N	1:B:132:ASP:OD1	2.52	0.42
1:B:352:VAL:HA	1:B:355:ILE:HG22	2.01	0.42
1:B:413:LEU:HD22	1:B:413:LEU:O	2.19	0.42
1:B:412:ILE:HG23	1:B:414:THR:HG23	2.02	0.42
1:E:238:TYR:OH	1:E:243:LEU:HD12	2.18	0.42
1:C:217:ARG:HG3	1:C:218:ILE:N	2.34	0.42
1:C:413:LEU:HG	1:C:416:LEU:HD21	2.01	0.42
1:E:84:GLU:OE1	1:E:85:PHE:HD2	2.01	0.42
1:A:422:HIS:O	1:A:425:PHE:HB2	2.20	0.42
1:E:60:PRO:HG2	1:E:212:GLU:HB3	2.01	0.42
1:C:94:LEU:O	1:C:98:VAL:HG23	2.20	0.42
1:D:425:PHE:HA	1:D:428:PHE:CD1	2.54	0.42
1:E:60:PRO:HB3	1:E:216:LEU:HD21	2.01	0.42
1:A:126:ARG:HD2	1:A:160:ILE:O	2.20	0.42
1:A:143:PRO:HA	1:A:193:LEU:HD22	2.01	0.42
1:B:262:LEU:O	1:B:266:ILE:HG13	2.19	0.42
1:C:130:LEU:O	1:C:134:VAL:HG23	2.19	0.42
1:C:361:CYS:C	1:C:362:TYR:HD1	2.22	0.42
1:A:132:ASP:O	1:A:136:MET:HG3	2.20	0.42
1:A:413:LEU:HA	1:A:416:LEU:HG	2.02	0.42
1:B:255:ASP:HB3	1:B:258:ALA:HB3	2.00	0.42
1:C:402:LEU:HD21	1:C:424:LEU:HD23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:291:GLN:OE1	1:D:340:GLN:N	2.42	0.42
1:B:294:ASN:OD1	1:B:296:LYS:HB3	2.20	0.42
1:B:376:THR:HG21	1:B:401:LEU:HD21	2.02	0.42
1:D:365:ARG:NH1	1:D:368:TYR:OH	2.53	0.42
1:E:86:ALA:O	1:E:87:LYS:CB	2.67	0.42
1:B:239:LYS:HE3	1:B:277:GLN:O	2.20	0.41
1:B:359:MET:CE	1:B:404:ILE:HG22	2.50	0.41
1:E:375:THR:O	1:E:379:ILE:HG13	2.20	0.41
1:A:460:ILE:O	1:A:464:VAL:HG22	2.20	0.41
1:A:464:VAL:O	1:A:468:ILE:HG13	2.19	0.41
1:A:457:VAL:O	1:A:461:MET:SD	2.78	0.41
1:C:104:ILE:HD12	1:C:104:ILE:H	1.84	0.41
1:C:151:ASN:HD22	1:C:151:ASN:C	2.24	0.41
1:C:455:ASP:O	1:C:459:SER:OG	2.36	0.41
1:E:398:LEU:O	1:E:402:LEU:HB2	2.20	0.41
1:E:468:ILE:O	1:E:468:ILE:HG22	2.21	0.41
1:B:150:ARG:HD3	1:B:190:MET:HG3	2.01	0.41
1:B:436:MET:O	1:B:440:VAL:HG23	2.20	0.41
1:D:20:ILE:HA	1:D:23:VAL:HG22	2.02	0.41
1:D:422:HIS:HA	1:D:425:PHE:CD2	2.56	0.41
1:E:84:GLU:OE1	1:E:84:GLU:C	2.58	0.41
1:A:85:PHE:HD2	1:A:91:VAL:HG13	1.86	0.41
1:B:404:ILE:O	1:B:408:THR:OG1	2.31	0.41
1:B:432:SER:HA	1:B:435:SER:OG	2.21	0.41
1:C:147:LEU:HD22	1:C:190:MET:HG2	2.03	0.41
1:C:163:ASP:OD1	1:C:164:GLU:N	2.47	0.41
1:D:154:LEU:HD22	1:D:226:ARG:HG3	2.03	0.41
1:D:440:VAL:HG23	1:D:463:LEU:HD13	2.03	0.41
1:E:372:VAL:HA	1:E:375:THR:OG1	2.21	0.41
1:C:464:VAL:HA	1:C:467:LEU:CD1	2.51	0.41
1:E:168:THR:HA	1:E:172:THR:HG21	2.03	0.41
1:B:296:LYS:HG2	1:B:300:ILE:HD12	2.02	0.41
1:E:197:MET:SD	1:E:216:LEU:HD12	2.61	0.41
1:E:456:GLN:OE1	1:E:456:GLN:HA	2.21	0.41
1:A:218:ILE:HD13	1:B:11:MET:HG3	2.02	0.40
1:D:464:VAL:O	1:D:468:ILE:HG13	2.21	0.40
1:B:412:ILE:HG22	1:B:414:THR:OG1	2.20	0.40
1:C:416:LEU:CD2	1:C:416:LEU:N	2.81	0.40
1:D:310:ALA:HB2	1:D:318:ILE:HD13	2.04	0.40
1:E:213:ARG:NH2	1:E:255:ASP:OD1	2.49	0.40
1:A:60:PRO:HG2	1:A:212:GLU:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:TYR:HA	1:A:242:VAL:HB	2.03	0.40
1:D:344:SER:O	1:D:348:VAL:HG23	2.20	0.40
1:B:103:ASN:HB2	1:B:106:PRO:HD2	2.03	0.40
1:C:105:ILE:HB	1:C:106:PRO:HD3	2.03	0.40
1:C:404:ILE:N	1:C:405:PRO:HD2	2.37	0.40
1:B:105:ILE:HB	1:B:106:PRO:HD3	2.04	0.40
1:D:415:VAL:O	1:D:418:LEU:HB2	2.21	0.40
1:E:215:GLU:O	1:E:218:ILE:HG12	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	425/462 (92%)	411 (97%)	14 (3%)	0	100	100
1	B	420/462 (91%)	399 (95%)	18 (4%)	3 (1%)	22	54
1	C	429/462 (93%)	409 (95%)	18 (4%)	2 (0%)	29	61
1	D	423/462 (92%)	408 (96%)	15 (4%)	0	100	100
1	E	409/462 (88%)	395 (97%)	12 (3%)	2 (0%)	29	61
All	All	2106/2310 (91%)	2022 (96%)	77 (4%)	7 (0%)	41	71

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	414	THR
1	E	87	LYS
1	B	168	THR
1	C	365	ARG
1	B	336	ILE
1	C	233	VAL

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Mol	Chain	Res	Type
1	E	242	VAL

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	399/424 (94%)	395 (99%)	4 (1%)	76	89
1	B	398/424 (94%)	383 (96%)	15 (4%)	33	64
1	C	403/424 (95%)	389 (96%)	14 (4%)	36	67
1	D	399/424 (94%)	392 (98%)	7 (2%)	59	80
1	E	390/424 (92%)	379 (97%)	11 (3%)	43	71
All	All	1989/2120 (94%)	1938 (97%)	51 (3%)	46	72

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LEU
1	A	365	ARG
1	A	461	MET
1	A	467	LEU
1	B	14	LYS
1	B	83	ASP
1	B	85	PHE
1	B	168	THR
1	B	175	ASP
1	B	197	MET
1	B	208	LYS
1	B	339	ARG
1	B	371	LYS
1	B	400	ARG
1	B	407	ASP
1	B	413	LEU
1	B	415	VAL
1	B	425	PHE

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Mol	Chain	Res	Type
1	B	439	TYR
1	C	85	PHE
1	C	99	GLN
1	C	124	GLN
1	C	151	ASN
1	C	204	ARG
1	C	254	ARG
1	C	344	SER
1	C	359	MET
1	C	380	PHE
1	C	400	ARG
1	C	431	GLU
1	C	433	ARG
1	C	459	SER
1	C	467	LEU
1	D	84	GLU
1	D	87	LYS
1	D	90	LYS
1	D	99	GLN
1	D	380	PHE
1	D	411	ASN
1	D	413	LEU
1	E	89	ARG
1	E	96	GLU
1	E	204	ARG
1	E	314	ASP
1	E	337	GLN
1	E	351	GLN
1	E	355	ILE
1	E	373	LEU
1	E	434	LYS
1	E	439	TYR
1	E	454	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	B	21	GLN
1	B	290	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

27 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	A	503	-	3,3,3	0.46	0	2,2,2	0.27	0
2	EDO	A	502	-	3,3,3	0.46	0	2,2,2	0.30	0
3	GOL	D	505	-	5,5,5	0.37	0	5,5,5	0.32	0
2	EDO	C	502	-	3,3,3	0.48	0	2,2,2	0.26	0
3	GOL	C	503	-	5,5,5	0.35	0	5,5,5	0.28	0
3	GOL	B	503	-	5,5,5	0.37	0	5,5,5	0.28	0
4	SO4	B	506	-	4,4,4	0.15	0	6,6,6	0.07	0
2	EDO	D	501	-	3,3,3	0.45	0	2,2,2	0.32	0
4	SO4	A	507	-	4,4,4	0.16	0	6,6,6	0.11	0
2	EDO	B	502	-	3,3,3	0.42	0	2,2,2	0.35	0
2	EDO	D	503	-	3,3,3	0.43	0	2,2,2	0.72	0
3	GOL	B	505	-	5,5,5	0.38	0	5,5,5	0.29	0
2	EDO	C	501	-	3,3,3	0.45	0	2,2,2	0.27	0
2	EDO	A	504	-	3,3,3	0.47	0	2,2,2	0.21	0
3	GOL	D	504	-	5,5,5	0.38	0	5,5,5	0.16	0
2	EDO	D	502	-	3,3,3	0.47	0	2,2,2	0.29	0
2	EDO	E	501	-	3,3,3	0.46	0	2,2,2	0.45	0
4	SO4	E	505	-	4,4,4	0.13	0	6,6,6	0.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
3	GOL	E	503	-	5,5,5	0.35	0	5,5,5	0.23	0
2	EDO	B	501	-	3,3,3	0.45	0	2,2,2	0.30	0
2	EDO	E	502	-	3,3,3	0.44	0	2,2,2	0.42	0
3	GOL	B	504	-	5,5,5	0.37	0	5,5,5	0.23	0
3	GOL	A	506	-	5,5,5	0.36	0	5,5,5	0.23	0
2	EDO	A	505	-	3,3,3	0.47	0	2,2,2	0.30	0
5	PG4	C	504	-	12,12,12	0.43	0	11,11,11	0.37	0
3	GOL	E	504	-	5,5,5	0.35	0	5,5,5	0.28	0
2	EDO	A	501	-	3,3,3	0.44	0	2,2,2	0.34	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	A	503	-	-	1/1/1/1	-
2	EDO	A	502	-	-	0/1/1/1	-
3	GOL	D	505	-	-	0/4/4/4	-
2	EDO	C	502	-	-	0/1/1/1	-
3	GOL	C	503	-	-	2/4/4/4	-
3	GOL	B	503	-	-	2/4/4/4	-
2	EDO	D	501	-	-	0/1/1/1	-
2	EDO	B	502	-	-	0/1/1/1	-
2	EDO	D	503	-	-	1/1/1/1	-
3	GOL	B	505	-	-	2/4/4/4	-
2	EDO	C	501	-	-	0/1/1/1	-
2	EDO	A	504	-	-	0/1/1/1	-
3	GOL	D	504	-	-	2/4/4/4	-
2	EDO	D	502	-	-	0/1/1/1	-
2	EDO	E	501	-	-	0/1/1/1	-
3	GOL	E	503	-	-	2/4/4/4	-
2	EDO	B	501	-	-	1/1/1/1	-
2	EDO	E	502	-	-	0/1/1/1	-
3	GOL	B	504	-	-	2/4/4/4	-
3	GOL	A	506	-	-	0/4/4/4	-
2	EDO	A	505	-	-	0/1/1/1	-
5	PG4	C	504	-	-	3/10/10/10	-
3	GOL	E	504	-	-	2/4/4/4	-
2	EDO	A	501	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	503	GOL	O1-C1-C2-C3
3	B	503	GOL	O1-C1-C2-C3
3	B	505	GOL	O1-C1-C2-C3
3	D	504	GOL	O1-C1-C2-O2
3	D	504	GOL	O1-C1-C2-C3
3	E	503	GOL	O1-C1-C2-C3
3	E	504	GOL	O1-C1-C2-C3
3	B	503	GOL	O1-C1-C2-O2
3	E	504	GOL	O1-C1-C2-O2
3	B	505	GOL	O1-C1-C2-O2
3	E	503	GOL	O1-C1-C2-O2
2	D	503	EDO	O1-C1-C2-O2
3	C	503	GOL	O1-C1-C2-O2
5	C	504	PG4	O2-C3-C4-O3
3	B	504	GOL	O1-C1-C2-O2
3	B	504	GOL	O1-C1-C2-C3
2	A	503	EDO	O1-C1-C2-O2
5	C	504	PG4	O1-C1-C2-O2
2	B	501	EDO	O1-C1-C2-O2
5	C	504	PG4	O4-C7-C8-O5

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	433/462 (93%)	-0.10	10 (2%)	60	37	15, 45, 104, 127	0
1	B	430/462 (93%)	-0.02	7 (1%)	72	51	14, 55, 101, 127	0
1	C	439/462 (95%)	0.19	20 (4%)	32	15	20, 63, 114, 129	0
1	D	433/462 (93%)	-0.01	7 (1%)	72	51	19, 51, 106, 122	0
1	E	423/462 (91%)	0.12	14 (3%)	46	24	14, 55, 107, 129	0
All	All	2158/2310 (93%)	0.04	58 (2%)	54	29	14, 53, 108, 129	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	410	ASN	4.6
1	A	441	LEU	3.5
1	E	340	GLN	3.4
1	C	314	ASP	3.3
1	D	430	TYR	3.3
1	C	434	LYS	3.2
1	E	315	GLY	2.9
1	C	386	GLU	2.9
1	C	172	THR	2.8
1	C	344	SER	2.8
1	A	168	THR	2.8
1	B	168	THR	2.7
1	E	207	GLU	2.7
1	C	458	ASP	2.7
1	B	460	ILE	2.7
1	E	443	ASN	2.7
1	E	400	ARG	2.7
1	E	309	PHE	2.7
1	C	168	THR	2.7
1	A	430	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	355	ILE	2.6
1	A	434	LYS	2.5
1	E	253	CYS	2.5
1	C	174	GLY	2.5
1	A	170	GLU	2.5
1	A	443	ASN	2.4
1	C	207	GLU	2.4
1	D	171	GLU	2.4
1	B	462	ASN	2.4
1	B	463	LEU	2.4
1	A	214	GLN	2.4
1	B	464	VAL	2.4
1	D	441	LEU	2.4
1	A	410	ASN	2.3
1	C	165	GLY	2.3
1	A	437	SER	2.3
1	C	421	PHE	2.3
1	C	460	ILE	2.2
1	C	469	GLN	2.2
1	D	440	VAL	2.2
1	C	208	LYS	2.2
1	C	170	GLU	2.2
1	A	460	ILE	2.2
1	E	463	LEU	2.1
1	B	461	MET	2.1
1	E	87	LYS	2.1
1	E	202	HIS	2.1
1	C	411	ASN	2.1
1	E	98	VAL	2.1
1	B	424	LEU	2.1
1	C	440	VAL	2.1
1	D	417	LYS	2.1
1	E	418	LEU	2.1
1	C	420	HIS	2.1
1	D	437	SER	2.0
1	E	83	ASP	2.0
1	D	379	ILE	2.0
1	C	254	ARG	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	EDO	C	501	4/4	0.66	0.38	48,64,85,85	0
3	GOL	E	503	6/6	0.75	0.26	33,54,78,86	0
2	EDO	D	502	4/4	0.77	0.33	58,77,95,95	0
2	EDO	C	502	4/4	0.78	0.38	44,85,103,103	0
2	EDO	A	502	4/4	0.78	0.38	65,78,81,96	0
2	EDO	A	504	4/4	0.80	0.19	34,51,73,73	0
3	GOL	B	503	6/6	0.81	0.25	50,79,103,103	0
2	EDO	E	501	4/4	0.83	0.25	47,66,82,82	0
3	GOL	A	506	6/6	0.83	0.35	46,63,75,80	0
3	GOL	D	504	6/6	0.84	0.26	56,75,92,92	0
5	PG4	C	504	13/13	0.84	0.21	48,72,86,95	0
2	EDO	A	505	4/4	0.85	0.21	50,74,88,88	0
2	EDO	E	502	4/4	0.86	0.29	37,46,56,59	0
3	GOL	D	505	6/6	0.86	0.20	52,69,84,84	0
3	GOL	E	504	6/6	0.87	0.20	56,72,90,102	0
3	GOL	C	503	6/6	0.91	0.22	51,61,74,89	0
3	GOL	B	504	6/6	0.91	0.26	44,61,83,99	0
3	GOL	B	505	6/6	0.91	0.21	46,60,83,93	0
2	EDO	A	501	4/4	0.91	0.31	51,62,75,83	0
4	SO4	B	506	5/5	0.92	0.21	46,55,86,92	0
2	EDO	D	501	4/4	0.92	0.15	46,57,68,78	0
4	SO4	A	507	5/5	0.92	0.20	54,63,89,99	0
4	SO4	E	505	5/5	0.92	0.18	59,64,70,76	0
2	EDO	B	501	4/4	0.94	0.20	39,53,64,67	0
2	EDO	D	503	4/4	0.94	0.23	27,32,42,42	0
2	EDO	A	503	4/4	0.94	0.20	32,40,63,63	0
2	EDO	B	502	4/4	0.94	0.22	39,47,56,56	0

6.5 Other polymers (i)

There are no such residues in this entry.