Full wwPDB X-ray Structure Validation Report (i)

Sep 6, 2023 – 08:33 PM EDT

PDB ID	:	4FVL
Title	:	Human collagenase 3 (MMP-13) full form with peptides from pro-domain
Authors	:	Stura, E.A.; Vera, L.; Visse, R.; Nagase, H.; Dive, V.
Deposited on	:	2012-06-29
Resolution	:	2.44 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:

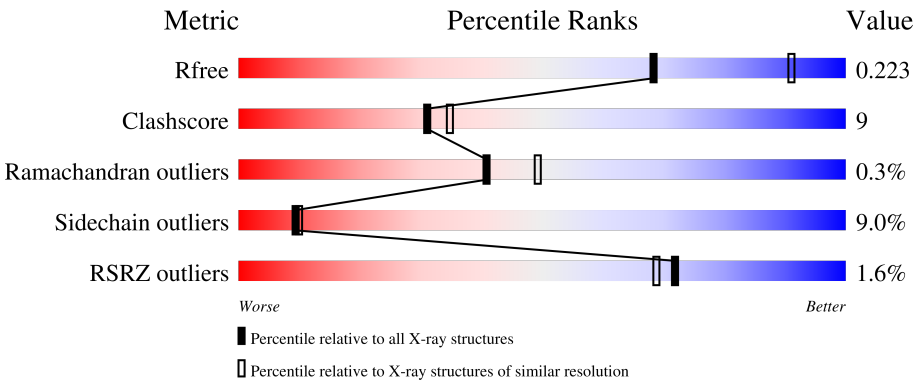
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.44 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	1564 (2.46-2.42)
Clashscore	141614	1631 (2.46-2.42)
Ramachandran outliers	138981	1617 (2.46-2.42)
Sidechain outliers	138945	1617 (2.46-2.42)
RSRZ outliers	127900	1547 (2.46-2.42)

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	368	% 76% 20% •
1	B	368	3% 81% 17% •
2	C	20	30% 35% 5% 30%
2	D	20	85% 15%

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
6	GOL	B	510	-	-	-	X
7	PGO	A	515	-	-	-	X
7	PGO	A	525	-	-	X	-
7	PGO	A	527	-	-	-	X
7	PGO	C	101	-	-	X	-
8	PEG	A	529	-	-	X	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 6842 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 Collagenase 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	368	3021	1961	495	555	10	0	3	0
1	B	368	2995	1945	492	548	10	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	223	ALA	GLU	engineered mutation	UNP P45452
B	223	ALA	GLU	engineered mutation	UNP P45452

- Molecule 2 is a protein called Collagenase 3, pro-domain peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	14	131	85	23	23	0	0	0
2	D	20	179	114	29	36	0	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
3	A	2	2	2	0	0
3	B	2	2	2	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
4	A	5	5	5	0	0

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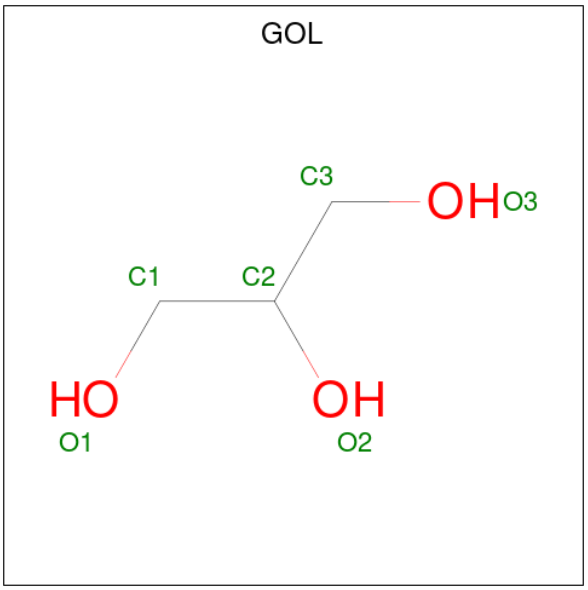
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
4	B	5	5	5	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
5	A	2	2	2	0	0
			Total	Cl		
5	B	1	1	1	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	A	1	6	3	3	0	0
			Total	C	O		
6	A	1	6	3	3	0	0
			Total	C	O		
6	A	1	6	3	3	0	0
			Total	C	O		
6	B	1	6	3	3	0	0
			Total	C	O		
6	B	1	6	3	3	0	0
			Total	C	O		
6	B	1	6	3	3	0	0

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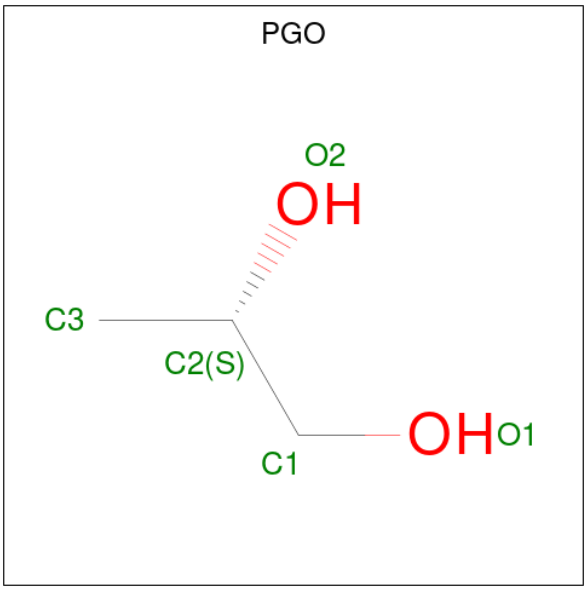
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	B	1	6	3	3	0	0
			Total	C	O		
6	B	1	6	3	3	0	0
			Total	C	O		
6	B	1	6	3	3	0	0
			Total	C	O		
6	B	1	6	3	3	0	0

- Molecule 7 is S-1,2-PROPANEDIOL (three-letter code: PGO) (formula: $C_3H_8O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	A	1	5	3	2	0	0
			Total	C	O		
7	A	1	5	3	2	0	0
			Total	C	O		
7	A	1	5	3	2	0	0
			Total	C	O		
7	A	1	5	3	2	0	0
			Total	C	O		
7	A	1	5	3	2	0	0
			Total	C	O		
7	A	1	5	3	2	0	0
			Total	C	O		
7	A	1	5	3	2	0	0

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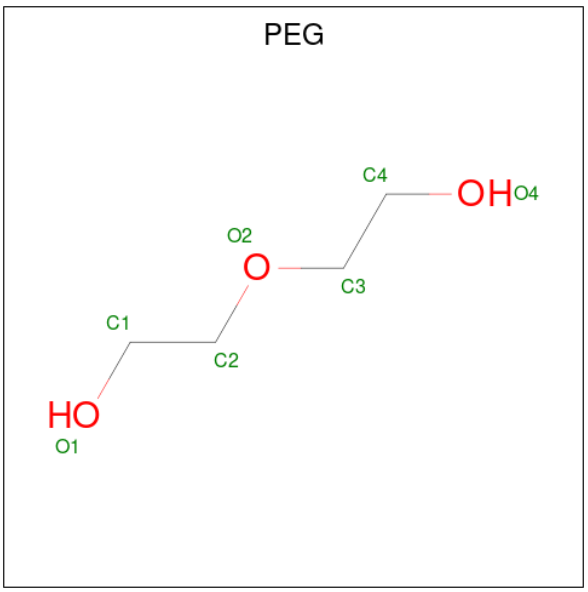
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
7	A	1	5	3	2		0	0
7	A	1	5	3	2		0	0
7	A	1	5	3	2		0	0
7	A	1	5	3	2		0	0
7	A	1	5	3	2		0	0
7	A	1	5	3	2		0	0
7	A	1	5	3	2		0	0
7	A	1	5	3	2		0	0
7	B	1	5	3	2		0	0
7	B	1	5	3	2		0	0
7	B	1	5	3	2		0	0
7	B	1	5	3	2		0	0
7	B	1	5	3	2		0	0
7	B	1	5	3	2		0	0
7	B	1	5	3	2		0	0
7	B	1	5	3	2		0	0
7	B	1	5	3	2		0	0
7	B	1	5	3	2		0	0
7	B	1	5	3	2		0	0
7	C	1	5	3	2		0	0

- Molecule 8 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
8	A	1	7	4	3	0	0
8	A	1	7	4	3	0	0
8	A	1	7	4	3	0	0
8	A	1	7	4	3	0	0
8	A	1	7	4	3	0	0
8	B	1	7	4	3	0	0
8	B	1	7	4	3	0	0
8	B	1	7	4	3	0	0
8	D	1	7	4	3	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	A	102	102	102	0	1
9	B	115	115	115	0	0

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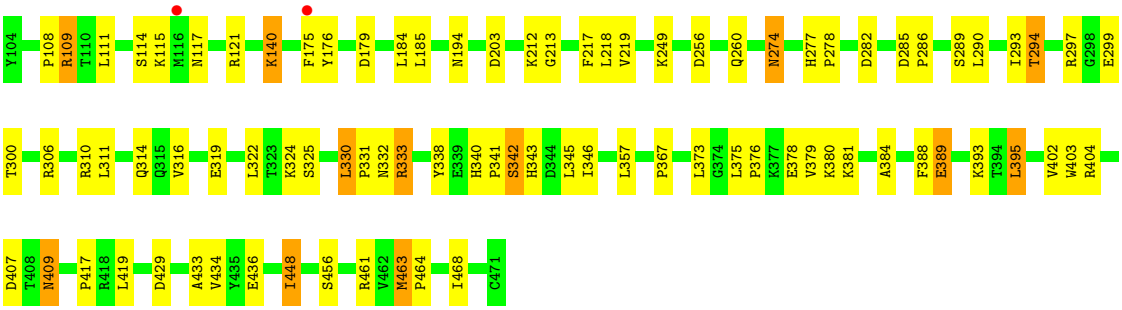
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	C	4	5	5	0	1
			Total	O		
9	D	13	14	14	0	1

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.

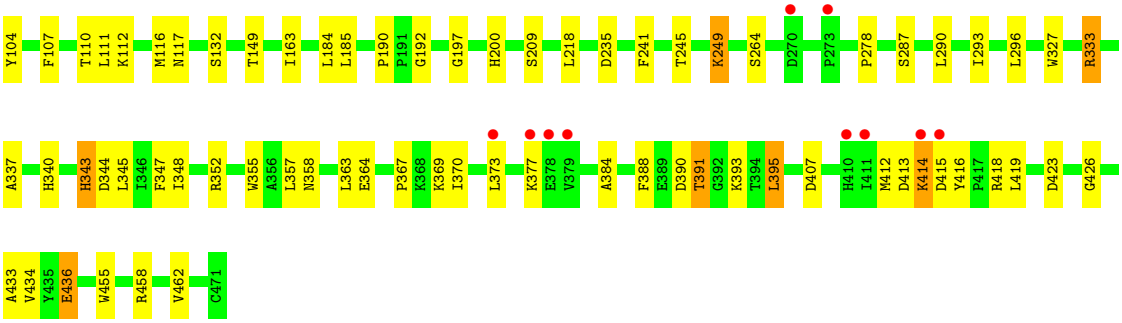
• Molecule 1: Collagenase 3

Chain A:



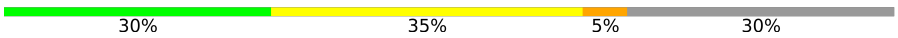
• Molecule 1: Collagenase 3

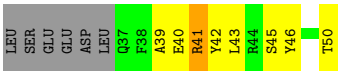
Chain B:



• Molecule 2: Collagenase 3, pro-domain peptide

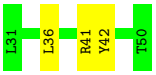
Chain C:





• Molecule 2: Collagenase 3, pro-domain peptide

Chain D:


L31
L36
R41
Y42
T50

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	125.78Å 157.27Å 105.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.11 – 2.44 49.11 – 2.44	Depositor EDS
% Data completeness (in resolution range)	95.8 (49.11-2.44) 95.8 (49.11-2.44)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	0.15	Depositor
$< I/\sigma(I) >$ [1]	1.34 (at 2.42Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.166 , 0.223 0.167 , 0.223	Depositor DCC
R_{free} test set	1891 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	33.1	Xtriage
Anisotropy	0.216	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 57.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6842	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% 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: GOL, ZN, CA, CL, PGO, PEG

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	0.44	0/3125	0.57	0/4245
1	B	0.44	0/3099	0.58	0/4210
2	C	0.40	0/136	0.66	0/182
2	D	0.42	0/184	0.58	0/247
All	All	0.44	0/6544	0.58	0/8884

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3021	0	2873	64	0
1	B	2995	0	2851	46	0
2	C	131	0	117	8	0
2	D	179	0	160	1	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
5	A	2	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	1	0	0	0	0
6	A	18	0	24	4	0
6	B	42	0	56	4	0
7	A	75	0	120	13	0
7	B	60	0	96	7	0
7	C	5	0	8	4	0
8	A	35	0	50	8	0
8	B	21	0	30	5	0
8	D	7	0	10	1	0
9	A	102	0	0	5	0
9	B	115	0	0	5	0
9	C	5	0	0	0	0
9	D	14	0	0	1	0
All	All	6842	0	6395	118	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 9.

All (118) 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)
6:B:515:GOL:H12	9:B:637:HOH:O	1.63	0.98
1:B:209:SER:HB2	6:B:509:GOL:H12	1.61	0.82
1:B:104:TYR:N	8:B:529:PEG:HO1	1.79	0.81
1:A:456:SER:OG	7:A:525:PGO:H11	1.81	0.80
1:A:456:SER:OG	7:A:525:PGO:C1	2.31	0.79
2:C:39:ALA:HA	2:C:41:ARG:HD3	1.68	0.76
1:B:343:HIS:HB3	1:B:345:LEU:HD23	1.71	0.72
1:A:429:ASP:OD2	1:B:458:ARG:NH2	2.24	0.71
1:A:332:ASN:HB2	8:A:529:PEG:H32	1.75	0.69
1:B:116:MET:SD	9:B:696:HOH:O	2.51	0.68
1:A:331:PRO:HB3	8:A:529:PEG:H41	1.76	0.67
1:B:245:THR:HA	8:B:528:PEG:H22	1.75	0.67
1:B:235:ASP:HA	7:B:516:PGO:H12	1.79	0.64
1:B:355:TRP:NE1	1:B:367:PRO:HG3	2.12	0.64
1:A:448:ILE:HB	1:B:462:VAL:HG11	1.80	0.63
1:B:414:LYS:O	1:B:416:TYR:N	2.33	0.61
1:B:190:PRO:HG2	2:D:42:TYR:HB3	1.83	0.61
1:A:184:LEU:HD22	2:C:45:SER:OG	2.01	0.60
1:A:388:PHE:HE1	1:A:395:LEU:HD22	1.67	0.60
1:B:426:GLY:H	6:B:512:GOL:H11	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:388:PHE:HB2	1:B:391:THR:HG22	1.84	0.59
1:B:249:LYS:HE2	1:B:249:LYS:H	1.67	0.59
1:A:367:PRO:HD2	7:A:527:PGO:H31	1.84	0.58
1:A:456:SER:CB	7:A:525:PGO:H11	2.34	0.57
1:A:330:LEU:HD21	1:A:357:LEU:HD11	1.88	0.56
1:A:140:LYS:NZ	6:A:510:GOL:O3	2.36	0.56
1:A:464:PRO:HD3	6:B:511:GOL:H2	1.88	0.55
2:C:39:ALA:HB2	7:C:101:PGO:O2	2.07	0.53
1:A:388:PHE:CE2	1:A:436:GLU:HG3	2.43	0.53
1:A:212:LYS:HD3	1:A:213:GLY:H	1.73	0.53
2:C:42:TYR:HE2	7:C:101:PGO:H33	1.74	0.53
1:B:235:ASP:HA	7:B:516:PGO:C1	2.38	0.53
1:A:448:ILE:HD13	1:A:463:MET:O	2.08	0.52
1:A:384:ALA:HB1	1:A:434:VAL:HG12	1.90	0.52
1:A:456:SER:OG	7:A:525:PGO:H12	2.08	0.52
1:A:294:THR:HG23	1:A:338:TYR:HA	1.92	0.51
1:A:289:SER:OG	6:A:512:GOL:H32	2.11	0.51
1:A:294:THR:HG23	5:A:509:CL:CL	2.48	0.51
1:B:241:PHE:CE2	8:B:530:PEG:H21	2.46	0.51
1:B:290:LEU:HD12	1:B:293:ILE:HD11	1.92	0.51
1:B:293:ILE:HG13	1:B:433:ALA:HB1	1.93	0.50
1:A:342:SER:N	1:A:389:GLU:OE1	2.44	0.50
1:A:333:ARG:NH2	9:A:690:HOH:O	2.45	0.50
8:B:529:PEG:H11	9:B:669:HOH:O	2.11	0.50
1:A:140:LYS:HZ1	6:A:510:GOL:C3	2.24	0.50
1:A:282:ASP:H	7:A:519:PGO:C1	2.23	0.50
1:A:256:ASP:OD2	1:A:260:GLN:NE2	2.40	0.50
2:C:39:ALA:HB1	2:C:42:TYR:HD2	1.76	0.49
1:A:322:LEU:O	1:A:325:SER:HB2	2.12	0.49
1:B:249:LYS:H	1:B:249:LYS:CD	2.25	0.49
1:B:384:ALA:HB1	1:B:434:VAL:HG12	1.95	0.49
1:A:409:ASN:OD1	1:A:409:ASN:N	2.46	0.49
1:A:332:ASN:H	8:A:529:PEG:H32	1.78	0.49
1:A:376:PRO:HG2	7:A:522:PGO:H12	1.95	0.48
1:A:249:LYS:HD2	1:A:249:LYS:H	1.78	0.48
1:A:417:PRO:HG3	7:A:522:PGO:H2	1.96	0.48
1:B:278:PRO:HG2	7:B:524:PGO:H31	1.96	0.48
7:A:524:PGO:H2	9:A:647:HOH:O	2.14	0.47
1:B:200:HIS:HE2	7:B:517:PGO:H12	1.78	0.47
1:B:249:LYS:H	1:B:249:LYS:CE	2.28	0.47
1:A:319:GLU:OE1	9:A:607:HOH:O	2.20	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:LEU:HD12	1:A:379:VAL:HG21	1.96	0.47
1:A:108:PRO:HD3	9:A:702:HOH:O	2.15	0.47
1:A:290:LEU:O	6:A:512:GOL:H31	2.14	0.47
1:A:388:PHE:CE1	1:A:395:LEU:HD22	2.48	0.47
8:A:528:PEG:H22	9:A:654:HOH:O	2.14	0.47
1:B:412:MET:HE3	1:B:412:MET:HA	1.98	0.46
1:B:192:GLY:HA2	7:B:521:PGO:H32	1.98	0.46
1:A:175:PHE:HB2	1:A:176:TYR:CE1	2.50	0.46
1:A:179:ASP:OD1	1:A:179:ASP:N	2.46	0.46
2:C:42:TYR:CE2	7:C:101:PGO:H33	2.51	0.46
1:B:388:PHE:CE2	1:B:436:GLU:HG3	2.51	0.46
1:A:341:PRO:HD3	7:A:524:PGO:H11	1.96	0.46
1:A:341:PRO:CD	7:A:524:PGO:H11	2.46	0.46
1:B:249:LYS:NZ	9:B:665:HOH:O	2.27	0.45
2:C:41:ARG:HH21	7:C:101:PGO:H11	1.82	0.45
8:D:101:PEG:H42	9:D:210:HOH:O	2.16	0.45
1:A:140:LYS:HD2	1:A:217:PHE:CE1	2.51	0.45
1:A:324:LYS:NZ	8:A:529:PEG:H11	2.32	0.45
1:A:393:LYS:HD3	1:A:404:ARG:HD2	1.97	0.45
1:B:241:PHE:CD2	8:B:530:PEG:H21	2.52	0.45
1:B:200:HIS:HE2	7:B:517:PGO:C1	2.30	0.44
1:A:378:GLU:OE2	1:A:378:GLU:N	2.38	0.44
1:B:343:HIS:CB	1:B:345:LEU:HD23	2.42	0.44
1:B:388:PHE:HE1	1:B:395:LEU:HD22	1.82	0.44
1:A:299:GLU:OE1	1:A:310:ARG:HD3	2.18	0.43
1:B:290:LEU:CD1	1:B:293:ILE:HD11	2.48	0.43
1:B:369:LYS:HD3	1:B:369:LYS:HA	1.71	0.43
1:B:149:THR:O	7:B:519:PGO:O2	2.36	0.43
1:B:327:TRP:CD1	1:B:357:LEU:HD22	2.53	0.43
1:A:115:LYS:HD2	1:A:117:ASN:O	2.19	0.43
1:A:109:ARG:HD3	1:A:111:LEU:HD23	2.00	0.43
1:B:344:ASP:OD2	1:B:358:ASN:ND2	2.48	0.42
1:B:163:ILE:HG23	1:B:197:GLY:O	2.19	0.42
1:B:414:LYS:C	1:B:416:TYR:H	2.21	0.42
1:A:219:VAL:HG13	2:C:46:TYR:HD2	1.84	0.42
1:A:274:ASN:N	1:A:274:ASN:OD1	2.53	0.42
1:A:314:GLN:OE1	8:A:532:PEG:H12	2.20	0.42
1:A:140:LYS:HB3	1:A:217:PHE:CD1	2.55	0.42
1:B:333:ARG:NH2	9:B:615:HOH:O	2.49	0.42
1:B:391:THR:HG23	1:B:393:LYS:H	1.84	0.42
1:A:403:TRP:CE2	1:A:417:PRO:HB3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:LEU:CD1	7:A:514:PGO:H11	2.49	0.42
1:B:352:ARG:O	1:B:370:ILE:HG23	2.20	0.41
1:A:293:ILE:HG13	1:A:433:ALA:HB1	2.03	0.41
1:A:300:THR:HG21	1:A:468:ILE:HD11	2.02	0.41
1:B:337:ALA:HA	1:B:347:PHE:O	2.19	0.41
1:B:112:LYS:HB3	1:B:112:LYS:HE2	1.91	0.41
1:A:332:ASN:H	8:A:529:PEG:C3	2.34	0.41
1:A:346:ILE:CG2	1:A:357:LEU:HB2	2.51	0.41
1:B:107:PHE:HB3	1:B:111:LEU:HD12	2.01	0.41
1:A:277:HIS:HA	1:A:278:PRO:HD3	1.93	0.41
1:A:343:HIS:O	1:A:345:LEU:HD13	2.21	0.40
1:A:285:ASP:HA	1:A:286:PRO:HD3	1.82	0.40
1:A:311:LEU:CD2	8:A:528:PEG:H11	2.51	0.40
1:A:456:SER:HB3	7:A:525:PGO:H11	2.03	0.40
1:B:393:LYS:NZ	1:B:413:ASP:OD2	2.44	0.40
1:A:286:PRO:HG2	1:B:287:SER:HB3	2.01	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	369/368 (100%)	356 (96%)	13 (4%)	0	100 100
1	B	366/368 (100%)	355 (97%)	9 (2%)	2 (0%)	29 34
2	C	12/20 (60%)	12 (100%)	0	0	100 100
2	D	18/20 (90%)	18 (100%)	0	0	100 100
All	All	765/776 (99%)	741 (97%)	22 (3%)	2 (0%)	41 49

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	415	ASP
1	B	414	LYS

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	325/322 (101%)	296 (91%)	29 (9%)	9 10
1	B	322/322 (100%)	296 (92%)	26 (8%)	11 13
2	C	13/19 (68%)	9 (69%)	4 (31%)	0 0
2	D	19/19 (100%)	17 (90%)	2 (10%)	7 6
All	All	679/682 (100%)	618 (91%)	61 (9%)	9 10

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	ARG
1	A	114	SER
1	A	121	ARG
1	A	140	LYS
1	A	185	LEU
1	A	194	ASN
1	A	203	ASP
1	A	218	LEU
1	A	274	ASN
1	A	294	THR
1	A	297	ARG
1	A	306	ARG
1	A	316	VAL
1	A	330	LEU
1	A	333	ARG
1	A	340	HIS
1	A	342	SER
1	A	373	LEU
1	A	380	LYS
1	A	381	LYS

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Mol	Chain	Res	Type
1	A	389	GLU
1	A	395	LEU
1	A	402	VAL
1	A	407	ASP
1	A	409	ASN
1	A	419	LEU
1	A	448	ILE
1	A	461	ARG
1	A	463	MET
1	B	110	THR
1	B	117	ASN
1	B	132	SER
1	B	184	LEU
1	B	185	LEU
1	B	218	LEU
1	B	249	LYS
1	B	264	SER
1	B	296	LEU
1	B	333	ARG
1	B	340	HIS
1	B	343	HIS
1	B	348	ILE
1	B	363	LEU
1	B	364	GLU
1	B	373	LEU
1	B	377	LYS
1	B	390	ASP
1	B	391	THR
1	B	395	LEU
1	B	407	ASP
1	B	418	ARG
1	B	419	LEU
1	B	423	ASP
1	B	436	GLU
1	B	455	TRP
2	C	40	GLU
2	C	41	ARG
2	C	43	LEU
2	C	50	THR
2	D	36	LEU
2	D	41	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are

no such sidechains identified.

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)

Of 64 ligands modelled in this entry, 17 are monoatomic - leaving 47 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	$\#\|Z\| > 2$
7	PGO	A	525	-	3,4,4	0.33	0	1,4,4	0.46	0
7	PGO	A	520	-	3,4,4	0.91	0	1,4,4	0.19	0
8	PEG	A	529	-	6,6,6	0.45	0	5,5,5	0.20	0
6	GOL	B	510	-	5,5,5	0.36	0	5,5,5	0.43	0
6	GOL	B	513	-	5,5,5	0.38	0	5,5,5	0.52	0
8	PEG	B	528	-	6,6,6	0.30	0	5,5,5	0.44	0
7	PGO	A	515	-	3,4,4	0.05	0	1,4,4	0.30	0
8	PEG	D	101	-	6,6,6	0.53	0	5,5,5	0.90	0
7	PGO	B	518	-	3,4,4	0.85	0	1,4,4	0.08	0
8	PEG	B	529	-	6,6,6	0.59	0	5,5,5	0.68	0
7	PGO	A	523	-	3,4,4	0.79	0	1,4,4	0.20	0
6	GOL	A	511	-	5,5,5	0.35	0	5,5,5	0.26	0
7	PGO	C	101	-	3,4,4	0.91	0	1,4,4	0.11	0
8	PEG	B	530	-	6,6,6	0.73	0	5,5,5	0.53	0
7	PGO	A	514	-	3,4,4	0.50	0	1,4,4	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	PGO	B	523	-	3,4,4	0.84	0	1,4,4	0.02	0
7	PGO	B	517	-	3,4,4	0.43	0	1,4,4	0.08	0
7	PGO	A	513	-	3,4,4	0.93	0	1,4,4	0.20	0
7	PGO	B	522	-	3,4,4	0.65	0	1,4,4	0.09	0
7	PGO	B	516	-	3,4,4	0.59	0	1,4,4	1.49	0
7	PGO	A	516	-	3,4,4	0.82	0	1,4,4	0.21	0
6	GOL	A	512	-	5,5,5	0.33	0	5,5,5	0.65	0
7	PGO	A	518	-	3,4,4	0.80	0	1,4,4	0.18	0
8	PEG	A	532	-	6,6,6	0.45	0	5,5,5	0.55	0
7	PGO	A	519	-	3,4,4	0.93	0	1,4,4	0.09	0
7	PGO	B	524	-	3,4,4	0.81	0	1,4,4	0.11	0
6	GOL	B	511	-	5,5,5	0.35	0	5,5,5	0.50	0
8	PEG	A	528	-	6,6,6	0.71	0	5,5,5	0.58	0
7	PGO	B	527	-	3,4,4	0.71	0	1,4,4	0.04	0
6	GOL	B	514	-	5,5,5	0.50	0	5,5,5	0.57	0
6	GOL	B	512	-	5,5,5	0.42	0	5,5,5	0.16	0
7	PGO	A	517	-	3,4,4	0.87	0	1,4,4	0.28	0
6	GOL	A	510	-	5,5,5	0.36	0	5,5,5	0.66	0
8	PEG	A	530	-	6,6,6	0.57	0	5,5,5	0.15	0
7	PGO	B	519	-	3,4,4	0.83	0	1,4,4	0.27	0
7	PGO	A	521	-	3,4,4	0.84	0	1,4,4	0.00	0
7	PGO	B	526	-	3,4,4	0.10	0	1,4,4	0.06	0
7	PGO	A	522	-	3,4,4	0.72	0	1,4,4	0.24	0
7	PGO	A	524	-	3,4,4	0.12	0	1,4,4	0.44	0
7	PGO	A	526	-	3,4,4	0.23	0	1,4,4	0.71	0
6	GOL	B	509	-	5,5,5	0.63	0	5,5,5	1.18	0
6	GOL	B	515	-	5,5,5	0.59	0	5,5,5	1.43	1 (20%)
8	PEG	A	531	-	6,6,6	0.62	0	5,5,5	0.29	0
7	PGO	B	520	-	3,4,4	0.80	0	1,4,4	0.10	0
7	PGO	B	521	-	3,4,4	0.85	0	1,4,4	0.13	0
7	PGO	A	527	-	3,4,4	0.78	0	1,4,4	0.16	0
7	PGO	B	525	-	3,4,4	0.31	0	1,4,4	0.38	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
7	PGO	A	525	-	-	0/2/2/2	-
7	PGO	A	520	-	-	0/2/2/2	-
8	PEG	A	529	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	B	510	-	-	2/4/4/4	-
6	GOL	B	513	-	-	2/4/4/4	-
8	PEG	B	528	-	-	4/4/4/4	-
7	PGO	A	515	-	-	2/2/2/2	-
8	PEG	D	101	-	-	1/4/4/4	-
7	PGO	B	518	-	-	2/2/2/2	-
8	PEG	B	529	-	-	4/4/4/4	-
7	PGO	A	523	-	-	2/2/2/2	-
6	GOL	A	511	-	-	0/4/4/4	-
7	PGO	C	101	-	-	0/2/2/2	-
8	PEG	B	530	-	-	2/4/4/4	-
7	PGO	A	514	-	-	1/2/2/2	-
7	PGO	B	523	-	-	2/2/2/2	-
7	PGO	B	517	-	-	0/2/2/2	-
7	PGO	A	513	-	-	0/2/2/2	-
7	PGO	B	522	-	-	0/2/2/2	-
7	PGO	B	516	-	-	2/2/2/2	-
7	PGO	A	516	-	-	0/2/2/2	-
6	GOL	A	512	-	-	4/4/4/4	-
7	PGO	A	518	-	-	0/2/2/2	-
8	PEG	A	532	-	-	2/4/4/4	-
7	PGO	A	519	-	-	0/2/2/2	-
7	PGO	B	524	-	-	0/2/2/2	-
6	GOL	B	511	-	-	2/4/4/4	-
8	PEG	A	528	-	-	3/4/4/4	-
7	PGO	B	527	-	-	1/2/2/2	-
6	GOL	B	514	-	-	2/4/4/4	-
6	GOL	B	512	-	-	2/4/4/4	-
7	PGO	A	517	-	-	0/2/2/2	-
6	GOL	A	510	-	-	2/4/4/4	-
8	PEG	A	530	-	-	2/4/4/4	-
7	PGO	B	519	-	-	2/2/2/2	-
7	PGO	A	521	-	-	1/2/2/2	-
7	PGO	B	526	-	-	1/2/2/2	-
7	PGO	A	522	-	-	0/2/2/2	-
7	PGO	A	524	-	-	2/2/2/2	-
7	PGO	A	526	-	-	1/2/2/2	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	B	509	-	-	2/4/4/4	-
6	GOL	B	515	-	-	2/4/4/4	-
8	PEG	A	531	-	-	1/4/4/4	-
7	PGO	B	520	-	-	0/2/2/2	-
7	PGO	B	521	-	-	0/2/2/2	-
7	PGO	A	527	-	-	0/2/2/2	-
7	PGO	B	525	-	-	2/2/2/2	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	515	GOL	C3-C2-C1	-2.41	102.34	111.70

There are no chirality outliers.

All (62) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	510	GOL	O1-C1-C2-C3
6	A	512	GOL	O1-C1-C2-C3
6	B	509	GOL	C1-C2-C3-O3
6	B	510	GOL	O1-C1-C2-C3
6	B	512	GOL	O1-C1-C2-O2
6	B	512	GOL	O1-C1-C2-C3
6	B	513	GOL	O1-C1-C2-C3
7	A	515	PGO	O1-C1-C2-C3
7	A	515	PGO	O1-C1-C2-O2
7	A	523	PGO	O1-C1-C2-C3
7	A	523	PGO	O1-C1-C2-O2
7	A	524	PGO	O1-C1-C2-C3
7	B	516	PGO	O1-C1-C2-C3
7	B	518	PGO	O1-C1-C2-C3
7	B	518	PGO	O1-C1-C2-O2
7	B	519	PGO	O1-C1-C2-O2
7	B	523	PGO	O1-C1-C2-O2
7	B	525	PGO	O1-C1-C2-C3
7	B	525	PGO	O1-C1-C2-O2
8	A	532	PEG	O2-C3-C4-O4
6	A	510	GOL	O1-C1-C2-O2
6	B	513	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
8	A	528	PEG	O1-C1-C2-O2
8	B	529	PEG	O1-C1-C2-O2
8	A	530	PEG	O1-C1-C2-O2
8	B	528	PEG	O1-C1-C2-O2
8	B	530	PEG	O2-C3-C4-O4
6	A	512	GOL	C1-C2-C3-O3
6	B	511	GOL	O1-C1-C2-C3
6	B	514	GOL	O1-C1-C2-C3
8	B	530	PEG	O1-C1-C2-O2
6	A	512	GOL	O1-C1-C2-O2
6	B	509	GOL	O2-C2-C3-O3
6	B	510	GOL	O1-C1-C2-O2
6	B	511	GOL	O1-C1-C2-O2
8	A	529	PEG	O2-C3-C4-O4
8	D	101	PEG	O1-C1-C2-O2
8	A	528	PEG	O2-C3-C4-O4
8	B	529	PEG	O2-C3-C4-O4
7	B	526	PGO	O1-C1-C2-O2
6	B	515	GOL	O1-C1-C2-O2
8	A	529	PEG	O1-C1-C2-O2
8	A	531	PEG	O2-C3-C4-O4
8	B	528	PEG	C1-C2-O2-C3
8	A	530	PEG	C4-C3-O2-C2
7	A	514	PGO	O1-C1-C2-C3
7	B	519	PGO	O1-C1-C2-C3
7	B	523	PGO	O1-C1-C2-C3
8	A	528	PEG	C4-C3-O2-C2
8	B	528	PEG	C4-C3-O2-C2
6	A	512	GOL	O2-C2-C3-O3
7	A	526	PGO	O1-C1-C2-O2
7	B	516	PGO	O1-C1-C2-O2
8	B	529	PEG	C1-C2-O2-C3
8	A	532	PEG	C4-C3-O2-C2
8	B	529	PEG	C4-C3-O2-C2
6	B	514	GOL	O1-C1-C2-O2
6	B	515	GOL	O1-C1-C2-C3
8	B	528	PEG	O2-C3-C4-O4
7	A	521	PGO	O1-C1-C2-O2
7	A	524	PGO	O1-C1-C2-O2
7	B	527	PGO	O1-C1-C2-O2

There are no ring outliers.

25 monomers are involved in 46 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	525	PGO	5	0
8	A	529	PEG	5	0
8	B	528	PEG	1	0
8	D	101	PEG	1	0
8	B	529	PEG	2	0
7	C	101	PGO	4	0
8	B	530	PEG	2	0
7	A	514	PGO	1	0
7	B	517	PGO	2	0
7	B	516	PGO	2	0
6	A	512	GOL	2	0
8	A	532	PEG	1	0
7	A	519	PGO	1	0
7	B	524	PGO	1	0
6	B	511	GOL	1	0
8	A	528	PEG	2	0
6	B	512	GOL	1	0
6	A	510	GOL	2	0
7	B	519	PGO	1	0
7	A	522	PGO	2	0
7	A	524	PGO	3	0
6	B	509	GOL	1	0
6	B	515	GOL	1	0
7	B	521	PGO	1	0
7	A	527	PGO	1	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	368/368 (100%)	-0.31	2 (0%)	91	91	15, 33, 56, 71	0
1	B	368/368 (100%)	-0.17	10 (2%)	54	50	16, 30, 63, 81	0
2	C	14/20 (70%)	0.06	0	100	100	27, 44, 82, 82	0
2	D	20/20 (100%)	-0.24	0	100	100	21, 38, 59, 61	0
All	All	770/776 (99%)	-0.24	12 (1%)	72	69	15, 32, 61, 82	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	273	PRO	4.5
1	B	270	ASP	3.5
1	B	410	HIS	2.9
1	B	379	VAL	2.9
1	B	415	ASP	2.9
1	A	175	PHE	2.8
1	B	378	GLU	2.4
1	B	373	LEU	2.4
1	B	414	LYS	2.3
1	A	116	MET	2.1
1	B	411	ILE	2.1
1	B	377	LYS	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 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
6	GOL	B	510	6/6	0.57	0.42	66,70,74,75	0
6	GOL	A	511	6/6	0.68	0.28	61,63,75,76	0
7	PGO	B	517	5/5	0.74	0.30	39,40,47,55	0
7	PGO	A	527	5/5	0.75	0.45	42,61,71,72	0
7	PGO	B	516	5/5	0.77	0.32	37,39,53,55	0
7	PGO	A	515	5/5	0.78	0.52	69,73,75,76	0
7	PGO	B	519	5/5	0.78	0.34	41,48,51,55	0
6	GOL	B	513	6/6	0.79	0.26	54,62,65,68	0
7	PGO	B	527	5/5	0.79	0.27	51,57,59,59	0
7	PGO	C	101	5/5	0.79	0.28	62,65,74,90	0
8	PEG	A	528	7/7	0.80	0.28	31,38,51,52	0
7	PGO	A	526	5/5	0.82	0.26	48,55,63,66	0
6	GOL	B	514	6/6	0.82	0.31	52,52,55,62	0
7	PGO	A	521	5/5	0.83	0.40	68,69,75,79	0
7	PGO	A	518	5/5	0.84	0.34	58,64,67,74	0
8	PEG	A	532	7/7	0.85	0.28	42,59,60,62	0
8	PEG	A	531	7/7	0.86	0.24	31,42,51,54	0
7	PGO	A	522	5/5	0.86	0.45	46,52,56,56	0
7	PGO	B	523	5/5	0.87	0.43	60,63,67,77	0
7	PGO	A	525	5/5	0.87	0.21	34,35,38,41	0
7	PGO	A	514	5/5	0.87	0.29	32,33,36,39	0
6	GOL	B	515	6/6	0.88	0.21	33,41,46,48	0
6	GOL	A	510	6/6	0.88	0.20	57,61,66,66	0
7	PGO	B	522	5/5	0.88	0.17	40,46,54,54	0
8	PEG	B	528	7/7	0.88	0.17	34,36,50,51	0
8	PEG	A	530	7/7	0.89	0.18	50,53,59,61	0
7	PGO	A	513	5/5	0.90	0.18	42,43,45,50	0
7	PGO	A	524	5/5	0.90	0.18	36,39,51,54	0
7	PGO	B	526	5/5	0.90	0.50	60,65,79,80	0
7	PGO	A	520	5/5	0.90	0.24	40,47,54,60	0
7	PGO	A	517	5/5	0.90	0.17	36,45,56,60	0
8	PEG	D	101	7/7	0.90	0.24	27,47,52,55	0
6	GOL	B	511	6/6	0.91	0.12	34,38,41,45	0
7	PGO	A	516	5/5	0.91	0.25	45,46,56,62	0
6	GOL	B	509	6/6	0.91	0.27	30,39,49,50	0
6	GOL	A	512	6/6	0.91	0.31	38,49,52,59	0
8	PEG	B	530	7/7	0.91	0.18	24,26,32,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	PEG	A	529	7/7	0.91	0.34	34,47,55,55	0
7	PGO	B	525	5/5	0.92	0.36	57,66,70,70	0
7	PGO	A	523	5/5	0.92	0.21	48,52,55,56	0
7	PGO	B	520	5/5	0.93	0.29	42,47,48,63	0
8	PEG	B	529	7/7	0.93	0.24	37,46,52,61	0
7	PGO	B	518	5/5	0.93	0.31	54,58,63,67	0
6	GOL	B	512	6/6	0.93	0.16	38,40,41,42	0
7	PGO	B	521	5/5	0.94	0.17	29,35,46,50	0
7	PGO	B	524	5/5	0.94	0.29	35,41,45,49	0
7	PGO	A	519	5/5	0.94	0.20	39,40,50,57	0
4	CA	B	507	1/1	0.96	0.06	47,47,47,47	0
4	CA	B	506	1/1	0.96	0.03	42,42,42,42	0
4	CA	A	507	1/1	0.97	0.07	55,55,55,55	0
5	CL	A	509	1/1	0.98	0.10	38,38,38,38	0
4	CA	A	506	1/1	0.98	0.04	34,34,34,34	0
4	CA	A	503	1/1	0.99	0.11	39,39,39,39	0
4	CA	B	505	1/1	0.99	0.15	25,25,25,25	0
4	CA	A	504	1/1	0.99	0.06	43,43,43,43	0
3	ZN	A	502	1/1	0.99	0.12	36,36,36,36	0
5	CL	B	508	1/1	1.00	0.09	21,21,21,21	0
4	CA	B	503	1/1	1.00	0.14	22,22,22,22	0
4	CA	B	504	1/1	1.00	0.09	28,28,28,28	0
3	ZN	B	501	1/1	1.00	0.16	19,19,19,19	0
4	CA	A	505	1/1	1.00	0.12	17,17,17,17	0
3	ZN	B	502	1/1	1.00	0.14	22,22,22,22	0
5	CL	A	508	1/1	1.00	0.11	14,14,14,14	0
3	ZN	A	501	1/1	1.00	0.14	24,24,24,24	0

6.5 Other polymers (i)

There are no such residues in this entry.