



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:07 PM GMT

PDB ID : 4H82
Title : Crystal structure of mutant MMP-9 catalytic domain in complex with a twin inhibitor.
Authors : Antoni, C.; Stura, E.A.; Vera, L.; Cassar-Lajeunesse, E.; Nuti, E.; Dive, V.; Rossello, A.
Deposited on : 2012-09-21
Resolution : 1.90 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

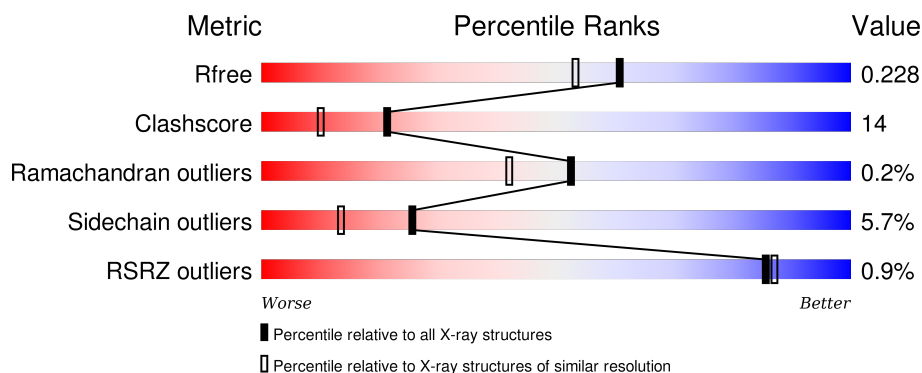
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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. 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	160	<div> <div>%</div> <div> <div></div> <div>66%</div> <div>31%</div> <div>.</div> </div> </div>
1	B	160	<div> <div>2%</div> <div> <div></div> <div>74%</div> <div>23%</div> <div>..</div> </div> </div>
1	C	160	<div> <div></div> <div> <div>66%</div> <div>31%</div> <div>..</div> </div> </div>
1	D	160	<div> <div>%</div> <div> <div></div> <div>66%</div> <div>33%</div> <div>..</div> </div> </div>

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6145 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 Matrix metalloproteinase-9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	160	Total	C	N	O	S	0	4	0
			1313	846	224	241	2			
1	B	160	Total	C	N	O	S	0	3	0
			1305	841	225	236	3			
1	C	160	Total	C	N	O	S	0	2	0
			1295	835	221	237	2			
1	D	160	Total	C	N	O	S	0	3	0
			1305	841	225	236	3			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	227	GLN	GLU	ENGINEERED MUTATION	UNP P14780
B	227	GLN	GLU	ENGINEERED MUTATION	UNP P14780
C	227	GLN	GLU	ENGINEERED MUTATION	UNP P14780
D	227	GLN	GLU	ENGINEERED MUTATION	UNP P14780

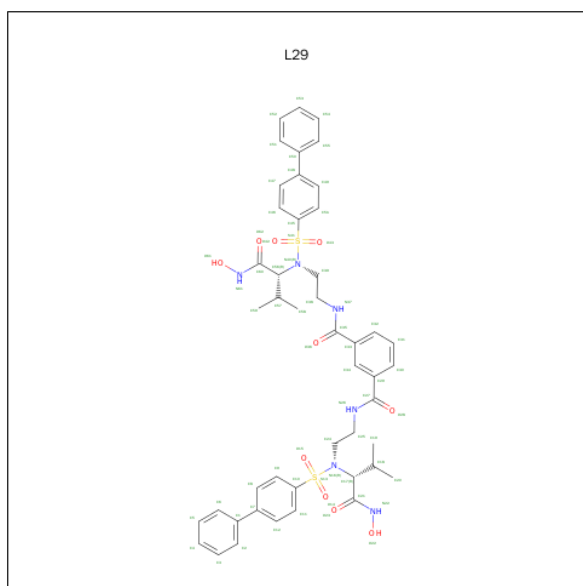
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 4 is N,N'-BIS(2-{(BIPHENYL-4-YLSULFONYL)}[(2R)-1-(HYDROXYAMINO)-3-METHYL-1-OXOBUTAN-2-YL]AMINO}ETHYL)BENZENE-1,3-DICARBOXAMIDE (NON-PREFERRED NAME) (three-letter code: L29) (formula: C₄₆H₅₂N₆O₁₀S₂).



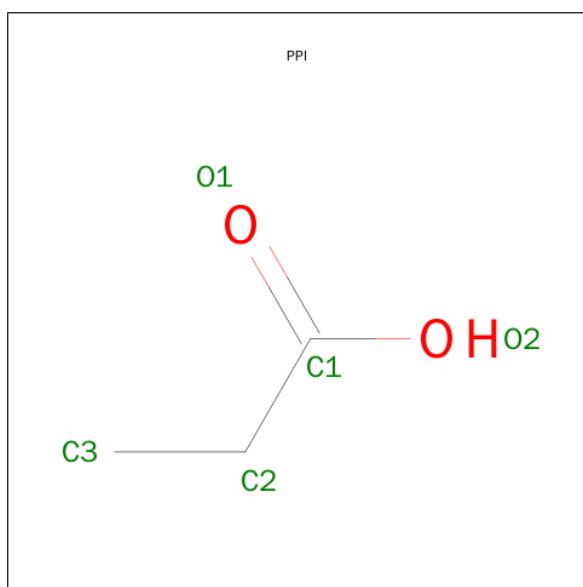
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O S 64 46 6 10 2	0	0
4	D	1	Total C N O S 64 46 6 10 2	0	0

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			7	4	3		
5	C	1	Total	C	O	0	0
			7	4	3		
5	C	1	Total	C	O	0	0
			7	4	3		
5	C	1	Total	C	O	0	0
			7	4	3		
5	C	1	Total	C	O	0	0
			7	4	3		
5	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is PROPANOIC ACID (three-letter code: PPI) (formula: C₃H₆O₂).



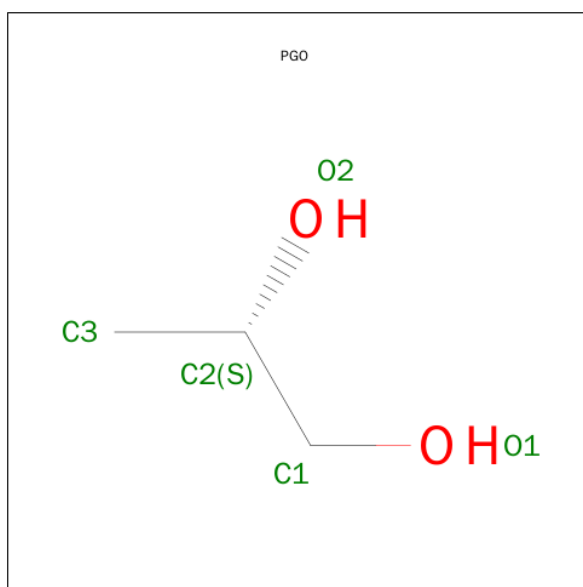
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			5	3	2		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 8 is S-1,2-PROPANEDIOL (three-letter code: PGO) (formula: $C_3H_8O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	D	1	Total	C	O	0	0
			5	3	2		
8	D	1	Total	C	O	0	0
			5	3	2		
8	D	1	Total	C	O	0	0
			5	3	2		

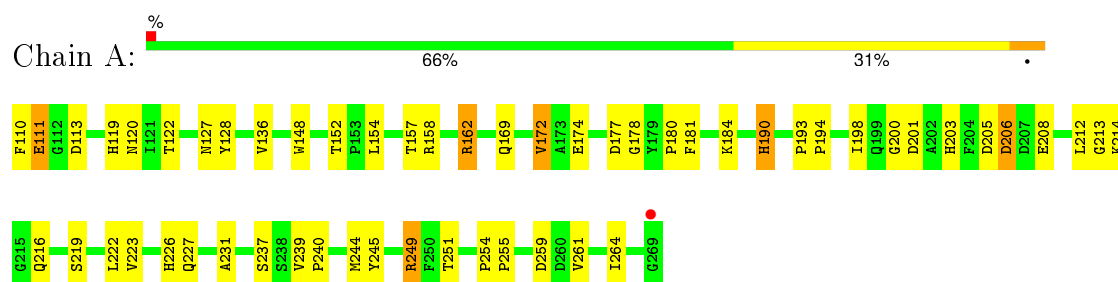
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	191	Total	O	0	1
			191	191		
9	D	171	Total	O	0	0
			171	171		
9	B	187	Total	O	0	0
			187	187		
9	C	155	Total	O	0	0
			155	155		

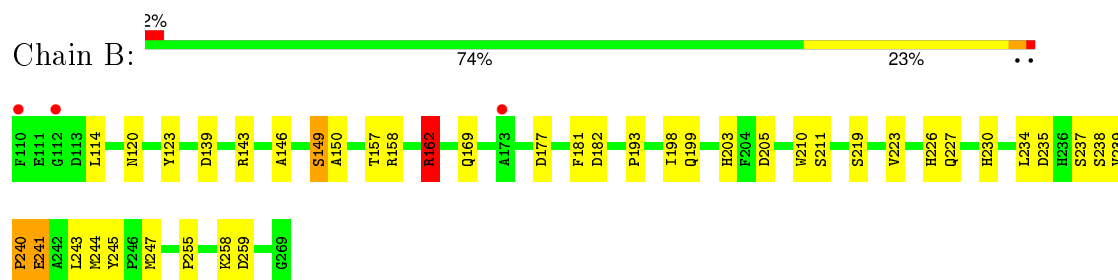
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

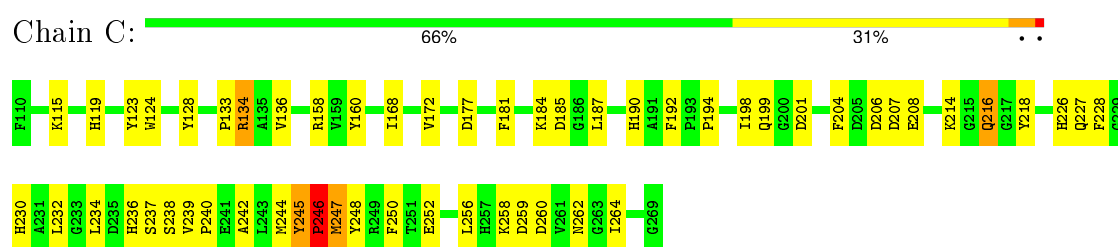
• Molecule 1: Matrix metalloproteinase-9



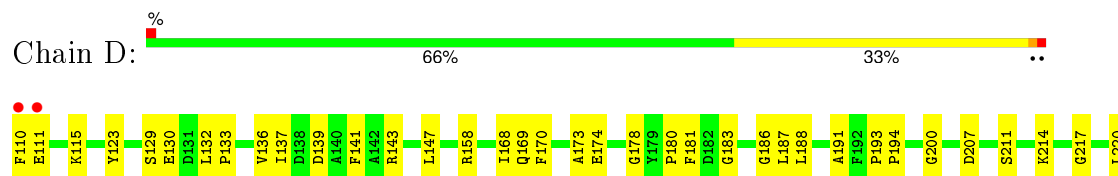
• Molecule 1: Matrix metalloproteinase-9

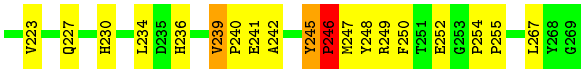


• Molecule 1: Matrix metalloproteinase-9



• Molecule 1: Matrix metalloproteinase-9





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	39.90 Å 98.86 Å 47.13 Å 90.03° 111.95° 89.98°	Depositor
Resolution (Å)	33.46 – 1.90 33.46 – 1.90	Depositor EDS
% Data completeness (in resolution range)	87.0 (33.46-1.90) 87.0 (33.46-1.90)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 1.91 Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8 _1069)	Depositor
R, R_{free}	0.207 , 0.241 0.203 , 0.228	Depositor DCC
R_{free} test set	2281 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	20.0	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 72.5	EDS
Estimated twinning fraction	0.480 for -h,k,-l 0.448 for -h,k,-l	Xtriage
Reported twinning fraction	0.480 for -h,k,-l	Depositor
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 45613 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6145	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.95 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.4757e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZN, PGO, CA, L29, PEG, PPI

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.38	0/1360	0.55	0/1850
1	B	0.40	0/1352	0.57	0/1839
1	C	0.43	1/1342 (0.1%)	0.61	1/1827 (0.1%)
1	D	0.43	1/1352 (0.1%)	0.58	1/1839 (0.1%)
All	All	0.41	2/5406 (0.0%)	0.58	2/7355 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	246	PRO	N-CD	5.17	1.55	1.47
1	D	246	PRO	N-CD	5.15	1.55	1.47

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	D	245	TYR	C-N-CD	5.68	140.33	128.40
1	C	245	TYR	C-N-CD	5.66	140.29	128.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	162[A]	ARG	Mainchain
1	C	134	ARG	Sidechain

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	1313	0	1207	39	0
1	B	1305	0	1205	29	0
1	C	1295	0	1190	42	2
1	D	1305	0	1205	37	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	3	0	0	0	0
4	A	64	0	50	2	0
4	D	64	0	50	7	0
5	C	42	0	60	2	0
5	D	7	0	10	0	0
6	C	5	0	5	0	0
7	C	6	0	8	2	0
8	D	15	0	24	2	0
9	A	191	0	0	5	0
9	B	187	0	0	5	1
9	C	155	0	0	13	0
9	D	171	0	0	2	2
All	All	6145	0	5014	148	3

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 14.

All (148) 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:C:214:LYS:HG3	7:C:312:GOL:H11	1.46	0.94
8:D:301:PGO:H31	9:D:558:HOH:O	1.80	0.81
1:A:136:VAL:HG13	1:A:212:LEU:HD11	1.69	0.75
4:D:303:L29:H22	4:D:303:L29:H17	1.68	0.75
1:C:187:LEU:HD11	9:D:447:HOH:O	1.88	0.73
1:D:174:GLU:HG3	1:D:180:PRO:HB3	1.74	0.69
1:C:239:VAL:HG12	9:C:527:HOH:O	1.92	0.68
1:C:239:VAL:CG1	9:C:527:HOH:O	2.42	0.67
1:A:120:ASN:OD1	1:A:157:THR:OG1	2.13	0.67
1:A:237:SER:OG	1:A:259:ASP:OD2	2.08	0.66
1:B:237:SER:OG	1:B:259:ASP:OD2	2.10	0.65
1:D:173:ALA:O	1:D:181:PHE:N	2.28	0.64
1:A:213:GLY:O	1:A:214:LYS:HB3	1.99	0.63
1:A:148:TRP:O	1:A:152:THR:OG1	2.14	0.62
1:A:169:GLN:NE2	9:A:465:HOH:O	2.32	0.62
1:A:205:ASP:HB3	1:A:208:GLU:HG2	1.82	0.62
1:C:234:LEU:HD11	1:C:264:ILE:HG12	1.81	0.61
1:C:240:PRO:HA	1:C:245:TYR:CD1	2.34	0.61
1:A:122:THR:HG22	1:A:157:THR:HB	1.81	0.61
1:C:236:HIS:CG	1:C:246:PRO:HB3	2.35	0.60
1:C:124:TRP:CD1	1:C:160:TYR:HA	2.37	0.60
1:A:128:TYR:OH	1:A:158:ARG:NH2	2.34	0.60
1:C:240:PRO:HA	1:C:245:TYR:CE1	2.39	0.58
1:D:132:LEU:HD21	1:D:211:SER:HA	1.85	0.58
1:C:258:LYS:HG3	9:C:457:HOH:O	2.05	0.57
1:C:230:HIS:ND1	1:C:234:LEU:O	2.36	0.57
1:B:120:ASN:HB3	9:B:424:HOH:O	2.04	0.57
1:A:222:LEU:HD11	1:A:251:THR:HG22	1.88	0.56
1:B:239:VAL:HG12	1:B:241:GLU:HG2	1.88	0.56
1:A:249[A]:ARG:NH2	9:A:540:HOH:O	2.39	0.55
1:D:248:TYR:O	1:D:249:ARG:HG2	2.08	0.54
1:C:192:PHE:HB2	1:C:199:GLN:HA	1.89	0.54
1:A:214:LYS:HG3	1:A:214:LYS:O	2.08	0.53
1:C:214:LYS:N	1:C:250:PHE:CZ	2.77	0.53
1:A:178:GLY:O	1:A:180:PRO:HD3	2.09	0.53
1:A:136:VAL:CG1	1:A:212:LEU:HD11	2.38	0.53
1:D:239:VAL:HG22	1:D:242:ALA:H	1.74	0.53
1:D:230:HIS:ND1	1:D:234:LEU:O	2.34	0.53
1:C:184:LYS:HE2	9:C:550:HOH:O	2.09	0.52
1:D:214:LYS:HG3	1:D:250:PHE:CE1	2.44	0.52
1:C:123:TYR:CZ	1:C:158:ARG:HB2	2.46	0.51
1:C:177:ASP:HB2	1:C:198:ILE:HD11	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:GLN:HG2	1:B:203:HIS:CD2	2.46	0.50
1:D:193:PRO:O	1:D:200:GLY:N	2.44	0.50
1:C:226:HIS:HA	1:C:244:MET:HE1	1.92	0.50
1:A:223:VAL:O	1:A:227:GLN:HG2	2.12	0.50
1:B:114:LEU:HD12	1:B:193:PRO:HB2	1.95	0.49
1:A:190:HIS:HB3	4:A:306:L29:H17	1.94	0.49
1:D:183:GLY:HA2	1:D:207:ASP:OD2	2.12	0.49
1:D:236:HIS:CE1	1:D:246:PRO:HB3	2.47	0.49
1:D:178:GLY:O	1:D:180:PRO:HD3	2.13	0.49
1:D:248:TYR:C	1:D:249:ARG:HG2	2.33	0.49
1:D:236:HIS:NE2	1:D:246:PRO:HB3	2.28	0.49
1:A:219:SER:HB3	1:A:222:LEU:HB2	1.93	0.49
1:C:237:SER:OG	1:C:259:ASP:OD2	2.28	0.48
1:C:237:SER:OG	5:C:313:PEG:H12	2.14	0.48
1:B:211:SER:O	1:B:219:SER:HA	2.13	0.48
1:D:115:LYS:HA	1:D:194:PRO:HG2	1.96	0.47
1:A:194:PRO:HG3	1:A:231:ALA:O	2.13	0.47
1:A:177:ASP:HB3	1:A:198:ILE:CD1	2.44	0.47
1:C:236:HIS:ND1	1:C:246:PRO:HB3	2.28	0.47
1:D:139:ASP:O	1:D:143:ARG:HG3	2.13	0.47
1:C:242:ALA:N	9:C:527:HOH:O	2.47	0.46
1:C:128:TYR:OH	1:C:158:ARG:NH2	2.48	0.46
1:C:198:ILE:O	1:C:201:ASP:HB2	2.16	0.46
1:A:190:HIS:CB	4:A:306:L29:H17	2.46	0.46
1:B:238:SER:O	1:B:240:PRO:HD3	2.16	0.46
1:A:240:PRO:HA	1:A:245:TYR:CD1	2.51	0.46
1:D:115:LYS:NZ	1:D:267:LEU:O	2.44	0.46
1:B:146:ALA:HA	1:B:149:SER:OG	2.16	0.46
1:B:258:LYS:HG3	9:B:417:HOH:O	2.15	0.45
1:D:137:ILE:HG23	1:D:220:LEU:HD21	1.97	0.45
1:D:188:LEU:N	4:D:303:L29:O43	2.42	0.45
1:A:198:ILE:HA	1:A:201:ASP:OD2	2.16	0.45
9:C:469:HOH:O	1:D:187:LEU:HD21	2.16	0.45
1:C:216:GLN:HA	9:C:540:HOH:O	2.16	0.45
1:B:123:TYR:CZ	1:B:158:ARG:HB2	2.51	0.45
1:B:169:GLN:NE2	9:B:473:HOH:O	2.44	0.45
1:A:240:PRO:HA	1:A:245:TYR:CG	2.52	0.45
1:A:162:ARG:NH1	9:A:548:HOH:O	2.48	0.44
1:B:210:TRP:CH2	1:B:223:VAL:HG11	2.52	0.44
1:D:230:HIS:CD2	4:D:303:L29:O61	2.70	0.44
1:B:150:ALA:N	9:B:573:HOH:O	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249[A]:ARG:NH1	1:B:182:ASP:OD2	2.51	0.44
1:D:191:ALA:HB2	1:D:227:GLN:HB3	2.00	0.44
1:C:115:LYS:HA	1:C:194:PRO:HG2	1.98	0.44
1:A:110:PHE:N	9:A:525:HOH:O	2.51	0.44
1:B:223:VAL:O	1:B:227:GLN:HG2	2.17	0.44
1:A:226:HIS:CE1	1:A:244:MET:HA	2.53	0.44
1:D:133:PRO:HB2	1:D:136:VAL:HG23	2.00	0.44
1:A:193:PRO:O	1:A:200:GLY:N	2.51	0.44
1:B:230:HIS:ND1	1:B:234:LEU:O	2.49	0.44
1:B:243:LEU:HB2	1:B:255:PRO:O	2.18	0.44
1:C:216:GLN:NE2	9:C:535:HOH:O	2.51	0.43
1:A:172:VAL:HG12	1:A:206:ASP:HB3	2.00	0.43
1:C:228:PHE:O	1:C:232:LEU:HG	2.19	0.43
1:C:214:LYS:HG3	7:C:312:GOL:C1	2.34	0.43
1:A:127:ASN:N	1:A:127:ASN:OD1	2.50	0.43
1:D:223:VAL:HG22	4:D:303:L29:H52	2.00	0.43
1:B:245:TYR:CE2	1:B:247:MET:HE3	2.53	0.43
1:C:245:TYR:CD2	1:C:247:MET:HB3	2.54	0.43
1:A:249[A]:ARG:NH2	1:B:182:ASP:OD2	2.51	0.42
1:C:133:PRO:O	1:C:136:VAL:HG22	2.19	0.42
1:D:129:SER:HB2	1:D:170:PHE:CD1	2.54	0.42
1:C:208:GLU:HG3	9:C:503:HOH:O	2.19	0.42
1:C:239:VAL:HG11	9:C:527:HOH:O	2.15	0.42
1:A:119:HIS:ND1	1:A:154:LEU:HD23	2.34	0.42
1:D:223:VAL:HG13	4:D:303:L29:H46	2.02	0.42
1:D:123:TYR:CZ	1:D:158:ARG:HB2	2.54	0.42
1:B:162[A]:ARG:H	1:B:162[A]:ARG:HG2	1.61	0.42
1:D:240:PRO:HA	1:D:245:TYR:CG	2.55	0.42
5:C:313:PEG:H42	9:C:509:HOH:O	2.20	0.42
1:C:181:PHE:CE1	1:C:190:HIS:CE1	3.07	0.42
4:D:303:L29:C46	4:D:303:L29:H33	2.50	0.42
1:A:169:GLN:O	1:A:203:HIS:HA	2.20	0.42
1:A:239:VAL:HA	1:A:240:PRO:HD3	1.91	0.42
1:B:255:PRO:HA	9:B:508:HOH:O	2.18	0.42
1:B:139:ASP:O	1:B:143:ARG:HG3	2.20	0.42
1:C:247:MET:HE2	1:D:186:GLY:HA2	2.01	0.42
1:C:226:HIS:HA	1:C:244:MET:CE	2.50	0.42
1:C:218:TYR:HD1	1:C:248:TYR:CE2	2.38	0.42
1:A:111[B]:GLU:HG3	9:A:587:HOH:O	2.19	0.41
1:A:181:PHE:HB3	1:A:205:ASP:OD2	2.20	0.41
1:D:147:LEU:HD21	1:D:255:PRO:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:HIS:HD1	1:B:244[B]:MET:HA	1.84	0.41
1:B:193:PRO:O	1:B:199:GLN:HB3	2.20	0.41
1:D:254:PRO:HA	1:D:255:PRO:HD3	1.72	0.41
1:D:240:PRO:HB2	1:D:241:GLU:OE1	2.20	0.41
1:C:185:ASP:N	1:C:208:GLU:OE2	2.54	0.41
1:A:254:PRO:HA	1:A:255:PRO:HD3	1.82	0.41
1:B:237:SER:O	1:B:245:TYR:HD1	2.03	0.41
1:D:239:VAL:HG22	1:D:241:GLU:H	1.85	0.41
1:B:226:HIS:HD2	1:B:227:GLN:NE2	2.18	0.41
1:D:141:PHE:CE2	1:D:168:ILE:HG21	2.56	0.41
1:C:192:PHE:CB	1:C:199:GLN:HA	2.51	0.41
1:A:261:VAL:O	1:A:264:ILE:HG22	2.20	0.41
1:D:217:GLY:O	8:D:310:PGO:H11	2.21	0.41
1:A:178:GLY:C	1:A:180:PRO:HD3	2.41	0.40
1:C:134:ARG:NH1	9:C:536:HOH:O	2.54	0.40
1:C:168:ILE:HG23	1:C:204:PHE:HE1	1.86	0.40
1:B:177:ASP:HB2	1:B:198:ILE:HD11	2.03	0.40
1:D:115:LYS:HB2	1:D:115:LYS:HE3	1.87	0.40
1:D:246:PRO:CG	4:D:303:L29:C34	2.99	0.40
1:B:181:PHE:HB3	1:B:205:ASP:OD2	2.21	0.40
1:B:240:PRO:HA	1:B:245:TYR:CD1	2.57	0.40
1:C:119:HIS:CE1	9:C:530:HOH:O	2.74	0.40
1:D:110:PHE:HB3	1:D:111:GLU:H	1.78	0.40
1:C:172:VAL:CG1	1:C:206:ASP:HB3	2.52	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:252:GLU:O	9:D:435:HOH:O[1_556]	2.00	0.20
9:B:472:HOH:O	9:B:513:HOH:O[1_655]	2.06	0.14
1:C:262:ASN:O	9:D:431:HOH:O[1_656]	2.11	0.09

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	162/160 (101%)	145 (90%)	17 (10%)	0	100	100
1	B	161/160 (101%)	145 (90%)	15 (9%)	1 (1%)	30	17
1	C	160/160 (100%)	151 (94%)	9 (6%)	0	100	100
1	D	161/160 (101%)	153 (95%)	8 (5%)	0	100	100
All	All	644/640 (101%)	594 (92%)	49 (8%)	1 (0%)	52	42

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	240	PRO

5.3.2 Protein sidechains ⓘ

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	132/128 (103%)	120 (91%)	12 (9%)	12	4
1	B	131/128 (102%)	125 (95%)	6 (5%)	33	21
1	C	130/128 (102%)	122 (94%)	8 (6%)	23	11
1	D	131/128 (102%)	125 (95%)	6 (5%)	33	21
All	All	524/512 (102%)	492 (94%)	32 (6%)	25	11

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

Mol	Chain	Res	Type
1	A	111[A]	GLU
1	A	111[B]	GLU
1	A	113	ASP
1	A	162	ARG
1	A	172	VAL
1	A	174	GLU
1	A	184	LYS

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Mol	Chain	Res	Type
1	A	190	HIS
1	A	206	ASP
1	A	216	GLN
1	A	249[A]	ARG
1	A	249[B]	ARG
1	B	149	SER
1	B	157	THR
1	B	162[A]	ARG
1	B	162[B]	ARG
1	B	235	ASP
1	B	241	GLU
1	C	207	ASP
1	C	216	GLN
1	C	227	GLN
1	C	238	SER
1	C	246	PRO
1	C	247	MET
1	C	256	LEU
1	C	260	ASP
1	D	130	GLU
1	D	169	GLN
1	D	239	VAL
1	D	246	PRO
1	D	247	MET
1	D	252	GLU

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

Mol	Chain	Res	Type
1	C	169	GLN
1	C	190	HIS
1	C	216	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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](#)

Of 34 ligands modelled in this entry, 20 are monoatomic - leaving 14 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	$\# Z > 2$
4	L29	A	306	2	66,68,68	5.55	35 (53%)	88,96,96	1.78	18 (20%)
5	PEG	C	306	-	6,6,6	0.42	0	5,5,5	0.12	0
5	PEG	C	307	-	6,6,6	0.75	0	5,5,5	1.37	0
6	PPI	C	308	-	1,4,4	0.46	0	0,4,4	0.00	-
5	PEG	C	309	-	6,6,6	0.54	0	5,5,5	1.49	0
5	PEG	C	310	-	6,6,6	0.72	0	5,5,5	1.15	0
5	PEG	C	311	-	6,6,6	0.50	0	5,5,5	0.71	0
7	GOL	C	312	-	5,5,5	0.72	0	5,5,5	0.74	0
5	PEG	C	313	-	6,6,6	0.65	0	5,5,5	1.34	0
8	PGO	D	301	-	4,4,4	0.38	0	2,4,4	0.90	0
4	L29	D	303	2	66,68,68	5.53	34 (51%)	88,96,96	2.25	24 (27%)
8	PGO	D	308	-	4,4,4	0.36	0	2,4,4	0.56	0
5	PEG	D	309	-	6,6,6	0.57	0	5,5,5	1.12	0
8	PGO	D	310	-	4,4,4	0.67	0	2,4,4	0.40	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
4	L29	A	306	2	-	0/80/80/80	0/5/5/5
5	PEG	C	306	-	-	0/4/4/4	0/0/0/0
5	PEG	C	307	-	-	0/4/4/4	0/0/0/0
6	PPI	C	308	-	-	0/0/2/2	0/0/0/0
5	PEG	C	309	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PEG	C	310	-	-	0/4/4/4	0/0/0/0
5	PEG	C	311	-	-	0/4/4/4	0/0/0/0
7	GOL	C	312	-	-	0/4/4/4	0/0/0/0
5	PEG	C	313	-	-	0/4/4/4	0/0/0/0
8	PGO	D	301	-	-	0/2/2/2	0/0/0/0
4	L29	D	303	2	-	0/80/80/80	0/5/5/5
8	PGO	D	308	-	-	0/2/2/2	0/0/0/0
5	PEG	D	309	-	-	0/4/4/4	0/0/0/0
8	PGO	D	310	-	-	0/2/2/2	0/0/0/0

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	306	L29	S13-N16	-4.55	1.56	1.63
4	D	303	L29	S13-N16	-2.92	1.58	1.63
4	D	303	L29	O23-C21	-2.39	1.18	1.23
4	A	306	L29	O28-C27	-2.25	1.18	1.23
4	A	306	L29	O23-C21	-2.21	1.19	1.23
4	D	303	L29	O28-C27	-2.08	1.19	1.23
4	A	306	L29	C51-C50	-2.01	1.34	1.39
4	A	306	L29	C53-C52	2.07	1.43	1.38
4	A	306	L29	C29-C27	2.20	1.54	1.50
4	D	303	L29	C8-C9	2.21	1.42	1.38
4	A	306	L29	C50-C48	2.23	1.54	1.49
4	D	303	L29	C29-C27	2.25	1.54	1.50
4	D	303	L29	C49-C48	2.47	1.44	1.39
4	D	303	L29	C50-C48	2.56	1.55	1.49
4	D	303	L29	C1-C7	2.57	1.55	1.49
4	D	303	L29	C33-C35	2.69	1.55	1.50
4	A	306	L29	C8-C9	2.71	1.43	1.38
4	A	306	L29	C1-C7	2.73	1.56	1.49
4	A	306	L29	C49-C48	2.76	1.45	1.39
4	D	303	L29	C52-C51	2.85	1.44	1.38
4	A	306	L29	C52-C51	2.90	1.44	1.38
4	A	306	L29	C49-C5A	3.28	1.44	1.38
4	D	303	L29	C49-C5A	3.39	1.44	1.38
4	A	306	L29	C47-C48	3.51	1.46	1.39
4	A	306	L29	C5-C6	3.61	1.46	1.38
4	D	303	L29	C5-C6	3.66	1.46	1.38
4	D	303	L29	C55-C50	3.75	1.47	1.39
4	A	306	L29	C55-C50	3.89	1.47	1.39
4	D	303	L29	C47-C48	3.94	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	306	L29	C34-C33	3.95	1.45	1.39
4	D	303	L29	C9-C10	4.11	1.45	1.38
4	A	306	L29	C9-C10	4.38	1.46	1.38
4	D	303	L29	C34-C33	4.65	1.46	1.39
4	D	303	L29	C10-S13	5.27	1.84	1.76
4	D	303	L29	C12-C11	5.37	1.48	1.38
4	A	306	L29	C45-S41	5.50	1.84	1.76
4	D	303	L29	C47-C46	5.64	1.48	1.38
4	A	306	L29	C12-C11	5.75	1.49	1.38
4	D	303	L29	C45-S41	5.77	1.85	1.76
4	A	306	L29	C11-C10	5.79	1.48	1.38
4	D	303	L29	C11-C10	5.79	1.48	1.38
4	A	306	L29	C47-C46	5.90	1.49	1.38
4	D	303	L29	C31-C30	5.93	1.51	1.38
4	D	303	L29	C35-N37	5.95	1.46	1.33
4	A	306	L29	C10-S13	5.98	1.85	1.76
4	A	306	L29	C31-C32	6.11	1.51	1.38
4	A	306	L29	C31-C30	6.12	1.51	1.38
4	D	303	L29	C8-C7	6.22	1.52	1.39
4	A	306	L29	C35-N37	6.38	1.47	1.33
4	A	306	L29	C8-C7	6.56	1.53	1.39
4	D	303	L29	C31-C32	6.63	1.52	1.38
4	A	306	L29	C3-C2	6.68	1.52	1.38
4	D	303	L29	C3-C2	6.80	1.52	1.38
4	D	303	L29	C27-N26	7.08	1.49	1.33
4	D	303	L29	S41-N40	7.08	1.73	1.63
4	A	306	L29	S41-N40	7.27	1.73	1.63
4	A	306	L29	C27-N26	7.29	1.49	1.33
4	D	303	L29	C5A-C45	8.04	1.52	1.38
4	A	306	L29	C5A-C45	8.12	1.52	1.38
4	A	306	L29	C34-C29	9.69	1.53	1.39
4	D	303	L29	C34-C29	10.41	1.54	1.39
4	A	306	L29	O42-S41	16.05	1.63	1.43
4	D	303	L29	O14-S13	16.35	1.64	1.43
4	D	303	L29	O42-S41	16.39	1.64	1.43
4	A	306	L29	O14-S13	16.43	1.64	1.43
4	A	306	L29	O43-S41	17.74	1.66	1.43
4	D	303	L29	O15-S13	18.16	1.66	1.43
4	D	303	L29	O43-S41	18.29	1.66	1.43
4	A	306	L29	O15-S13	18.79	1.67	1.43

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	303	L29	O14-S13-C10	-8.64	96.78	108.00
4	D	303	L29	O43-S41-O42	-8.26	105.22	119.47
4	A	306	L29	O43-S41-O42	-5.79	109.48	119.47
4	A	306	L29	O15-S13-C10	-5.75	100.53	108.00
4	D	303	L29	C39-N40-S41	-5.75	105.53	117.81
4	D	303	L29	C38-N37-C35	-4.46	112.15	122.15
4	D	303	L29	C9-C10-S13	-3.91	115.47	119.79
4	A	306	L29	O61-N61-C60	-3.81	114.48	119.86
4	A	306	L29	O14-S13-C10	-3.48	103.49	108.00
4	D	303	L29	O15-S13-C10	-3.04	104.05	108.00
4	D	303	L29	C10-S13-N16	-2.65	103.05	107.38
4	D	303	L29	O14-S13-O15	-2.23	115.62	119.47
4	A	306	L29	C38-N37-C35	-2.22	117.19	122.15
4	A	306	L29	O22-N22-C21	-2.15	116.83	119.86
4	D	303	L29	C18-C17-C21	-2.08	109.42	111.89
4	D	303	L29	C8-C7-C1	-2.02	117.77	121.39
4	D	303	L29	C58-C57-C56	2.01	116.45	110.82
4	A	306	L29	C39-C38-N37	2.05	115.46	111.72
4	D	303	L29	C39-C38-N37	2.07	115.49	111.72
4	A	306	L29	C30-C29-C34	2.14	121.83	119.24
4	D	303	L29	C21-C17-N16	2.14	116.10	110.35
4	D	303	L29	C20-C18-C17	2.15	116.83	110.82
4	D	303	L29	C24-C25-N26	2.18	115.69	111.72
4	D	303	L29	C45-S41-N40	2.23	111.03	107.38
4	A	306	L29	O14-S13-N16	2.33	111.93	106.97
4	A	306	L29	C56-C60-N61	2.36	120.44	115.56
4	D	303	L29	C30-C29-C34	2.40	122.14	119.24
4	A	306	L29	O62-C60-C56	2.41	125.35	121.34
4	A	306	L29	C32-C33-C34	2.54	122.31	119.24
4	A	306	L29	C19-C18-C17	2.56	118.00	110.82
4	D	303	L29	C59-C57-C56	2.60	118.11	110.82
4	A	306	L29	C60-C56-N40	2.75	117.73	110.35
4	D	303	L29	O43-S41-N40	2.86	113.05	106.97
4	D	303	L29	C60-C56-N40	3.27	119.13	110.35
4	D	303	L29	C11-C10-S13	3.30	123.43	119.79
4	A	306	L29	O43-S41-C45	3.48	112.53	108.00
4	A	306	L29	C38-C39-N40	3.49	118.35	112.34
4	D	303	L29	O15-S13-N16	3.89	115.24	106.97
4	A	306	L29	C25-C24-N16	4.25	119.64	112.34
4	D	303	L29	C25-C24-N16	4.40	119.90	112.34
4	A	306	L29	O15-S13-N16	4.82	117.21	106.97
4	D	303	L29	O14-S13-N16	5.17	117.94	106.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	306	L29	2	0
7	C	312	GOL	2	0
5	C	313	PEG	2	0
8	D	301	PGO	1	0
4	D	303	L29	7	0
8	D	310	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	160/160 (100%)	-0.11	1 (0%) 90 91	4, 13, 26, 44	0
1	B	160/160 (100%)	-0.12	3 (1%) 70 73	5, 12, 25, 68	0
1	C	160/160 (100%)	-0.17	0 100 100	6, 12, 26, 44	0
1	D	160/160 (100%)	-0.19	2 (1%) 79 82	6, 11, 22, 76	0
All	All	640/640 (100%)	-0.15	6 (0%) 85 87	4, 12, 26, 76	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	112	GLY	5.5
1	D	110	PHE	3.7
1	B	110	PHE	3.5
1	A	269	GLY	2.4
1	B	173	ALA	2.2
1	D	111	GLU	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. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
8	PGO	D	310	5/5	0.87	0.15	1.83	6,13,19,24	0
3	CA	A	305	1/1	0.97	0.12	1.45	39,39,39,39	0
3	CA	B	304	1/1	0.90	0.11	1.14	36,36,36,36	0
4	L29	D	303	64/64	0.95	0.10	0.13	1,10,21,26	0
4	L29	A	306	64/64	0.95	0.10	-0.26	3,9,18,24	0
8	PGO	D	301	5/5	0.95	0.11	-0.27	15,16,26,30	0
8	PGO	D	308	5/5	0.94	0.09	-0.83	5,7,9,12	0
3	CA	D	307	1/1	0.99	0.06	-1.11	13,13,13,13	0
3	CA	C	303	1/1	0.99	0.07	-1.43	8,8,8,8	0
2	ZN	D	302	1/1	1.00	0.07	-1.50	13,13,13,13	0
3	CA	B	302	1/1	1.00	0.05	-1.53	4,4,4,4	0
3	CA	C	305	1/1	0.96	0.06	-1.67	27,27,27,27	0
2	ZN	B	301	1/1	1.00	0.06	-2.18	22,22,22,22	0
2	ZN	A	302	1/1	0.99	0.06	-2.33	17,17,17,17	0
5	PEG	C	311	7/7	0.89	0.09	-2.56	8,19,23,27	0
3	CA	C	304	1/1	1.00	0.04	-2.89	10,10,10,10	0
3	CA	B	303	1/1	1.00	0.04	-3.14	12,12,12,12	0
3	CA	A	303	1/1	0.98	0.04	-3.28	9,9,9,9	0
3	CA	A	304	1/1	0.98	0.03	-4.00	25,25,25,25	0
3	CA	D	306	1/1	0.99	0.03	-4.39	22,22,22,22	0
3	CA	D	305	1/1	1.00	0.04	-4.80	15,15,15,15	0
2	ZN	C	302	1/1	0.99	0.05	-8.21	13,13,13,13	0
5	PEG	C	306	7/7	0.97	0.06	-	2,5,16,26	0
5	PEG	C	307	7/7	0.94	0.08	-	7,9,18,21	0
5	PEG	C	309	7/7	0.94	0.07	-	8,14,18,18	0
5	PEG	C	313	7/7	0.94	0.09	-	6,8,18,25	0
2	ZN	B	300	1/1	0.99	0.09	-	10,10,10,10	0
2	ZN	A	301	1/1	0.99	0.07	-	12,12,12,12	0
6	PPI	C	308	5/5	0.96	0.07	-	6,7,8,12	0
2	ZN	D	304	1/1	1.00	0.06	-	8,8,8,8	0
7	GOL	C	312	6/6	0.95	0.09	-	7,17,24,27	0
5	PEG	D	309	7/7	0.84	0.13	-	16,19,24,29	0
2	ZN	C	301	1/1	1.00	0.07	-	11,11,11,11	0
5	PEG	C	310	7/7	0.93	0.10	-	10,15,17,24	0

6.5 Other polymers

There are no such residues in this entry.