



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 10:31 pm BST

PDB ID : 4OR0
Title : Crystal Structure of Bovine Serum Albumin in complex with naproxen
Authors : Zielinski, K.; Bujacz, A.; Sekula, B.; Bujacz, G.
Deposited on : 2014-02-10
Resolution : 2.58 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

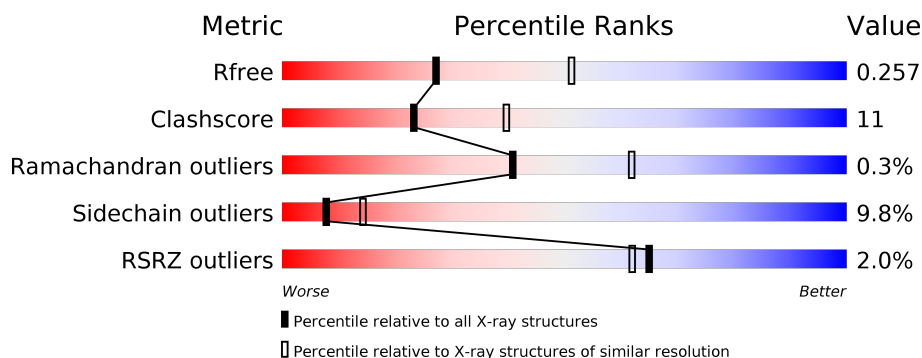
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.58 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	3676 (2.60-2.56)
Clashscore	141614	4049 (2.60-2.56)
Ramachandran outliers	138981	3979 (2.60-2.56)
Sidechain outliers	138945	3979 (2.60-2.56)
RSRZ outliers	127900	3614 (2.60-2.56)

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 $\leq 5\%$. 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	583	<div> <div>2%</div> <div> <div></div> <div>76%</div> <div>21%</div> <div>.</div> </div> </div>
1	B	583	<div> <div>2%</div> <div> <div></div> <div>68%</div> <div>28%</div> <div>.</div> </div> </div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9508 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.

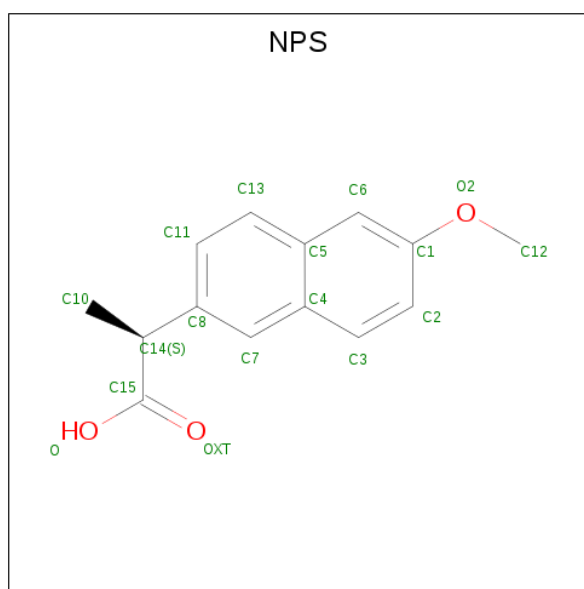
- Molecule 1 is a protein called Serum albumin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	582	Total	C	N	O	S	0	0	0
			4645	2931	780	895	39			
1	B	582	Total	C	N	O	S	0	0	0
			4645	2931	780	895	39			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	190	THR	ALA	VARIANT	UNP P02769
B	190	THR	ALA	VARIANT	UNP P02769

- Molecule 2 is (2S)-2-(6-methoxynaphthalen-2-yl)propanoic acid (three-letter code: NPS) (formula: C₁₄H₁₄O₃).



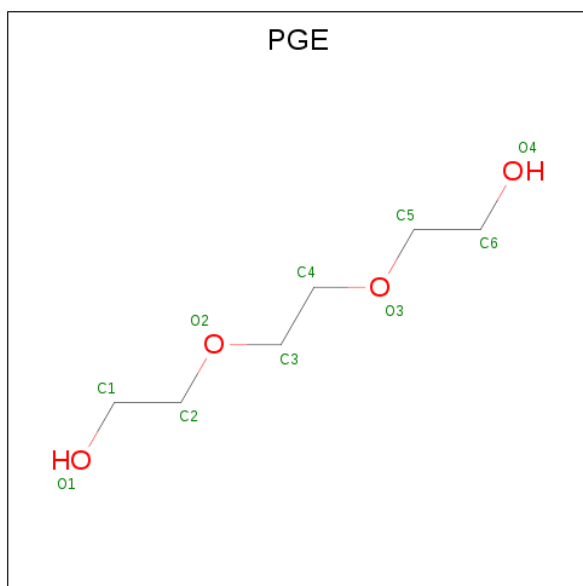
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			17	14	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			17	14	3		
2	A	1	Total	C	O	0	0
			17	14	3		
2	B	1	Total	C	O	0	0
			17	14	3		
2	B	1	Total	C	O	0	0
			17	14	3		
2	B	1	Total	C	O	0	0
			17	14	3		

- Molecule 3 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

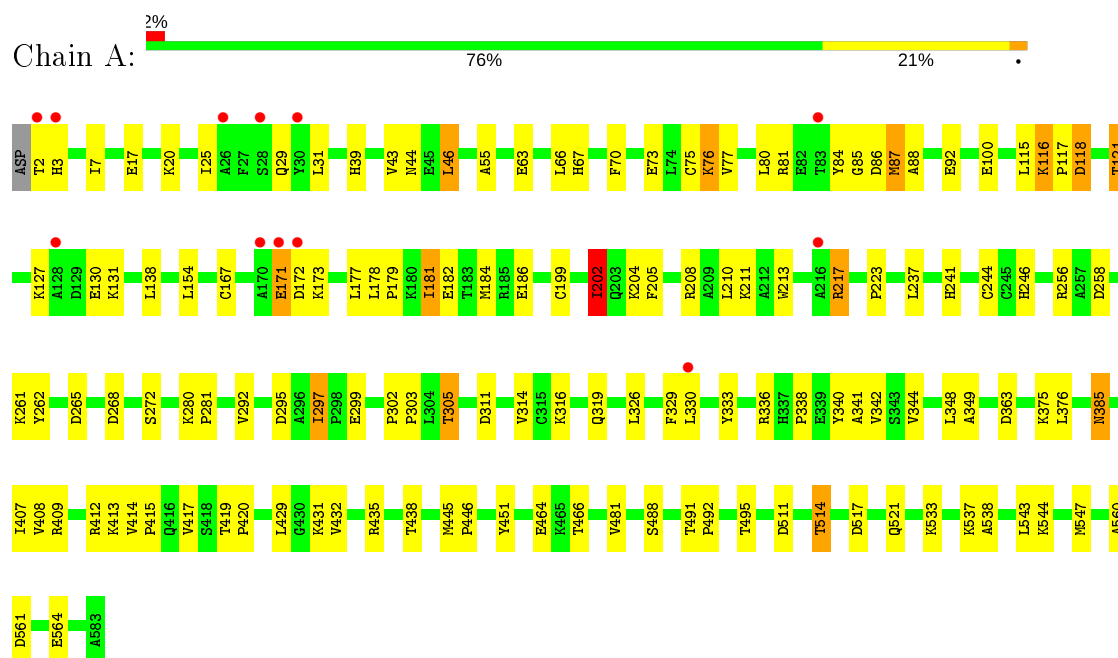
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	54	Total	O	0	0
			54	54		
5	B	45	Total	O	0	0
			45	45		

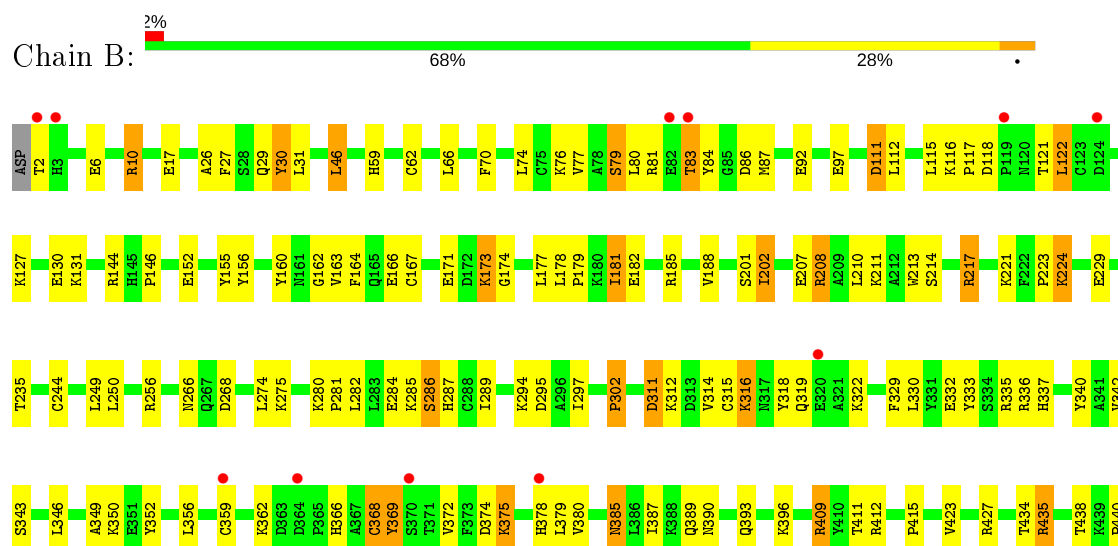
3 Residue-property plots [i](#)

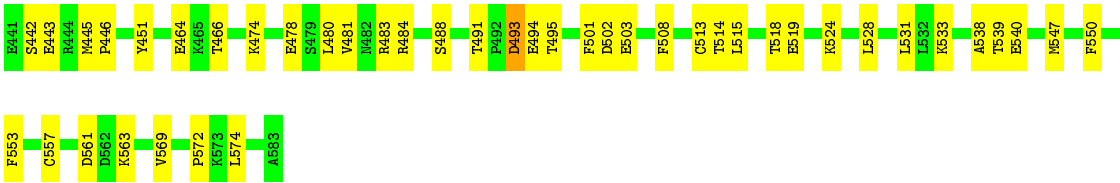
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Serum albumin



• Molecule 1: Serum albumin





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	216.04Å 44.90Å 141.70Å 90.00° 113.99° 90.00°	Depositor
Resolution (Å)	42.28 – 2.58 22.12 – 2.58	Depositor EDS
% Data completeness (in resolution range)	99.1 (42.28-2.58) 99.3 (22.12-2.58)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 2.56Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.183 , 0.257 0.185 , 0.257	Depositor DCC
R_{free} test set	1244 reflections (3.14%)	wwPDB-VP
Wilson B-factor (Å ²)	58.1	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 28.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9508	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, PGE, NPS

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	0.95	0/4740	1.01	5/6399 (0.1%)
1	B	0.89	3/4740 (0.1%)	0.98	4/6399 (0.1%)
All	All	0.92	3/9480 (0.0%)	1.00	9/12798 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	519	GLU	CD-OE2	5.38	1.31	1.25
1	B	79	SER	CB-OG	5.17	1.49	1.42
1	B	519	GLU	CG-CD	5.02	1.59	1.51

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	429	LEU	CB-CG-CD1	-5.58	101.51	111.00
1	B	547	MET	CA-CB-CG	5.47	122.60	113.30
1	A	75	CYS	CA-CB-SG	-5.45	104.19	114.00
1	B	502	ASP	CB-CG-OD2	5.32	123.09	118.30
1	A	154	LEU	CA-CB-CG	5.32	127.53	115.30
1	B	515	LEU	CB-CG-CD1	-5.32	101.96	111.00
1	A	202	ILE	CB-CA-C	-5.30	100.99	111.60
1	A	256	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	B	10	ARG	NE-CZ-NH1	5.06	122.83	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4645	0	4559	81	0
1	B	4645	0	4559	126	0
2	A	51	0	39	2	0
2	B	51	0	39	6	0
3	A	10	0	13	0	0
4	A	7	0	10	2	0
5	A	54	0	0	11	0
5	B	45	0	0	13	0
All	All	9508	0	9219	210	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (210) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:ILE:HG22	5:A:732:HOH:O	1.57	1.04
1:B:474:LYS:O	1:B:478:GLU:HG2	1.72	0.90
1:B:208:ARG:NH1	2:B:602:NPS:H2	1.88	0.89
1:B:202:ILE:CD1	1:B:210:LEU:HD22	2.06	0.86
1:B:202:ILE:HD11	1:B:210:LEU:HD22	1.57	0.84
1:A:297:ILE:H	1:A:297:ILE:HD13	1.40	0.84
1:B:280:LYS:HG2	1:B:281:PRO:HD2	1.59	0.83
1:A:330:LEU:HD13	1:A:349:ALA:HB2	1.60	0.83
1:B:26:ALA:HB2	1:B:249:LEU:HD12	1.60	0.82
1:A:432:VAL:HG12	2:A:601:NPS:H122	1.61	0.80
1:B:451:TYR:HD2	5:B:715:HOH:O	1.67	0.78
1:A:451:TYR:HD2	5:A:715:HOH:O	1.66	0.77
1:B:451:TYR:CD2	5:B:715:HOH:O	2.39	0.76
1:A:116:LYS:HA	1:A:116:LYS:HE2	1.68	0.75
1:B:217:ARG:HH21	1:B:342:VAL:HG21	1.52	0.74
1:B:81:ARG:HB2	5:B:745:HOH:O	1.86	0.73
1:B:224:LYS:HG2	5:B:731:HOH:O	1.89	0.72
1:A:451:TYR:CD2	5:A:715:HOH:O	2.40	0.72
1:A:385:ASN:N	1:A:385:ASN:OD1	2.14	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:LEU:HD21	1:A:87:MET:HE1	1.72	0.70
1:A:297:ILE:HD13	1:A:297:ILE:N	2.07	0.70
1:B:302:PRO:O	1:B:336:ARG:NH1	2.25	0.70
1:B:493:ASP:HB3	5:B:740:HOH:O	1.91	0.70
1:B:375:LYS:O	1:B:378:HIS:HB3	1.92	0.69
1:A:31:LEU:HD21	1:A:87:MET:CE	2.23	0.68
1:A:543:LEU:O	1:A:547:MET:HG3	1.97	0.65
1:B:181:ILE:HG22	1:B:182:GLU:N	2.10	0.65
1:A:280:LYS:HG2	1:A:281:PRO:HD2	1.77	0.65
1:A:435:ARG:NH2	5:A:715:HOH:O	2.30	0.64
1:A:181:ILE:CG2	5:A:732:HOH:O	2.27	0.62
1:B:202:ILE:HD11	1:B:210:LEU:CD2	2.29	0.62
1:B:332:GLU:O	1:B:335:ARG:HG2	2.01	0.60
1:B:229:GLU:OE2	1:B:229:GLU:HA	2.02	0.59
1:B:256:ARG:CZ	1:B:286:SER:HB3	2.32	0.59
1:B:368:CYS:SG	1:B:369:TYR:N	2.76	0.59
1:B:508:PHE:CZ	1:B:550:PHE:HE1	2.21	0.59
1:B:208:ARG:NH1	2:B:602:NPS:C2	2.64	0.59
1:B:217:ARG:HH21	1:B:342:VAL:CG2	2.16	0.59
1:A:297:ILE:HD11	1:A:338:PRO:HG3	1.85	0.58
1:B:97:GLU:OE2	1:B:97:GLU:N	2.32	0.58
1:A:435:ARG:HD2	1:A:451:TYR:CZ	2.39	0.58
1:B:329:PHE:HE2	1:B:349:ALA:HA	1.69	0.57
1:B:29:GLN:HG2	1:B:146:PRO:HA	1.86	0.57
1:A:25:ILE:O	1:A:29:GLN:HG3	2.03	0.57
1:B:557:CYS:O	1:B:563:LYS:HG2	2.04	0.57
1:B:316:LYS:CD	1:B:316:LYS:H	2.17	0.57
1:A:20:LYS:NZ	1:A:44:ASN:OD1	2.36	0.56
1:A:118:ASP:HB2	1:A:121:THR:OG1	2.04	0.56
1:A:55:ALA:HB3	5:A:754:HOH:O	2.05	0.56
1:B:359:CYS:O	1:B:362:LYS:HB2	2.05	0.56
1:A:81:ARG:HE	1:A:88:ALA:HB3	1.70	0.56
1:A:39:HIS:O	1:A:43:VAL:HG23	2.06	0.56
1:B:316:LYS:CD	1:B:316:LYS:N	2.68	0.56
1:A:25:ILE:HD11	1:A:138:LEU:HD22	1.88	0.55
1:A:408:VAL:O	1:A:412:ARG:HG3	2.07	0.55
1:B:329:PHE:CE2	1:B:349:ALA:HA	2.42	0.55
1:B:493:ASP:CB	5:B:740:HOH:O	2.52	0.55
1:B:508:PHE:CZ	1:B:550:PHE:CE1	2.96	0.54
1:B:435:ARG:HD2	1:B:451:TYR:CE2	2.41	0.54
1:B:318:TYR:CZ	1:B:322:LYS:HD3	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:LYS:HE2	1:B:174:GLY:H	1.73	0.54
1:B:412:ARG:NH2	1:B:538:ALA:O	2.41	0.54
1:B:171:GLU:OE2	1:B:171:GLU:N	2.41	0.54
1:B:167:CYS:HB3	1:B:177:LEU:HD21	1.90	0.53
1:B:330:LEU:HD13	1:B:349:ALA:HB2	1.90	0.53
1:B:480:LEU:HD12	1:B:483:ARG:CZ	2.38	0.53
1:B:280:LYS:CG	1:B:281:PRO:HD2	2.33	0.53
1:B:337:HIS:HB3	1:B:340:TYR:CD1	2.43	0.53
1:A:297:ILE:CD1	1:A:297:ILE:N	2.71	0.53
1:A:246:HIS:CE1	5:A:744:HOH:O	2.61	0.53
1:B:285:LYS:O	1:B:289:ILE:HG13	2.09	0.53
1:B:66:LEU:O	1:B:70:PHE:HD2	1.91	0.52
1:B:83:THR:HB	1:B:84:TYR:CD2	2.44	0.52
1:B:27:PHE:HD2	1:B:74:LEU:HD21	1.75	0.52
1:B:315:CYS:O	1:B:319:GLN:NE2	2.42	0.52
1:A:341:ALA:HB3	1:A:344:VAL:HG23	1.91	0.52
1:A:31:LEU:HD22	1:A:84:TYR:CZ	2.44	0.51
1:A:302:PRO:O	1:A:336:ARG:NH1	2.44	0.51
1:B:81:ARG:CB	5:B:745:HOH:O	2.53	0.51
1:A:415:PRO:O	1:A:533:LYS:HE2	2.11	0.51
1:B:311:ASP:HB3	1:B:314:VAL:HG23	1.93	0.51
1:B:77:VAL:HB	1:B:80:LEU:HD13	1.93	0.51
1:A:172:ASP:HA	5:A:731:HOH:O	2.10	0.51
1:A:63:GLU:OE2	1:A:63:GLU:N	2.36	0.51
1:B:316:LYS:N	1:B:316:LYS:HD2	2.27	0.50
1:A:213:TRP:CZ2	1:A:217:ARG:HD2	2.46	0.50
1:B:569:VAL:O	1:B:572:PRO:HD2	2.11	0.50
1:A:115:LEU:O	1:A:117:PRO:HD3	2.12	0.50
1:B:474:LYS:O	1:B:478:GLU:CG	2.54	0.50
1:B:185:ARG:NH1	5:B:730:HOH:O	2.44	0.50
1:B:160:TYR:O	1:B:164:PHE:HD2	1.95	0.49
1:A:171:GLU:CD	1:A:171:GLU:H	2.15	0.49
1:A:181:ILE:HG22	1:A:182:GLU:N	2.26	0.49
1:B:112:LEU:HD12	1:B:144:ARG:HG2	1.94	0.49
1:B:390:ASN:O	1:B:393:GLN:HB3	2.13	0.49
1:A:537:LYS:O	1:A:538:ALA:C	2.49	0.48
1:B:202:ILE:CD1	1:B:210:LEU:CD2	2.86	0.48
1:B:342:VAL:HG12	1:B:346:LEU:HD12	1.94	0.48
1:B:346:LEU:HD13	2:B:603:NPS:H123	1.95	0.48
1:B:77:VAL:HB	1:B:80:LEU:CD1	2.43	0.48
1:A:560:ALA:HB1	5:A:750:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:GLU:OE1	1:A:186:GLU:HA	2.13	0.48
1:B:162:GLY:O	1:B:166:GLU:HB3	2.13	0.48
1:B:372:VAL:HA	1:B:375:LYS:HG3	1.96	0.48
1:B:524:LYS:HE2	1:B:550:PHE:HE2	1.78	0.48
1:A:414:VAL:HB	1:A:417:VAL:HG23	1.95	0.48
1:B:178:LEU:N	1:B:179:PRO:CD	2.76	0.48
1:A:363:ASP:OD1	1:A:363:ASP:N	2.47	0.47
1:A:31:LEU:CD2	1:A:87:MET:HE2	2.44	0.47
1:A:31:LEU:CD2	1:A:87:MET:CE	2.92	0.47
1:B:378:HIS:HD2	5:B:743:HOH:O	1.98	0.47
1:B:316:LYS:H	1:B:316:LYS:HD3	1.80	0.47
1:A:261:LYS:HG3	1:A:262:TYR:N	2.30	0.46
1:B:210:LEU:O	1:B:213:TRP:HB3	2.15	0.46
1:B:369:TYR:O	1:B:372:VAL:HB	2.15	0.46
1:A:329:PHE:CE2	1:A:349:ALA:HA	2.51	0.46
1:B:379:LEU:HA	1:B:379:LEU:HD23	1.77	0.46
1:A:303:PRO:HB2	1:A:305:THR:OG1	2.14	0.46
1:A:217:ARG:HE	1:A:342:VAL:HG21	1.80	0.46
1:A:491:THR:HB	1:A:492:PRO:HD2	1.98	0.46
1:B:332:GLU:OE1	1:B:332:GLU:HA	2.15	0.46
1:B:440:PRO:HB2	1:B:443:GLU:HG3	1.97	0.46
1:B:484:ARG:HB2	5:B:733:HOH:O	2.16	0.46
1:A:223:PRO:HD2	1:A:295:ASP:HB3	1.98	0.45
1:B:451:TYR:HB3	5:B:715:HOH:O	2.16	0.45
1:A:199:CYS:HA	1:A:202:ILE:CD1	2.46	0.45
1:B:488:SER:HA	2:B:601:NPS:O	2.17	0.45
1:A:333:TYR:CZ	1:A:348:LEU:HD13	2.51	0.45
1:B:211:LYS:O	1:B:214:SER:HB2	2.17	0.45
1:B:6:GLU:OE2	1:B:10:ARG:NE	2.42	0.45
1:B:167:CYS:HB3	1:B:177:LEU:CD2	2.47	0.45
1:A:31:LEU:HD23	1:A:31:LEU:HA	1.64	0.45
1:B:26:ALA:CB	1:B:249:LEU:HD12	2.42	0.45
1:A:204:LYS:HB2	1:A:205:PHE:CD2	2.51	0.44
1:B:223:PRO:HD2	1:B:295:ASP:HB3	2.00	0.44
1:B:163:VAL:HG12	1:B:164:PHE:CD2	2.52	0.44
1:B:167:CYS:CB	1:B:177:LEU:HD21	2.46	0.44
1:A:202:ILE:CG1	1:A:210:LEU:HD22	2.48	0.44
1:A:311:ASP:O	1:A:314:VAL:HG23	2.17	0.44
1:B:59:HIS:HB3	1:B:62:CYS:SG	2.57	0.44
1:B:156:TYR:CD2	1:B:188:VAL:HG22	2.52	0.44
1:B:280:LYS:HD2	1:B:284:GLU:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:ASP:HA	1:A:261:LYS:HG2	2.00	0.44
1:B:202:ILE:CG1	1:B:210:LEU:HD22	2.47	0.44
1:A:76:LYS:HD3	1:A:76:LYS:N	2.33	0.44
1:B:508:PHE:CE2	1:B:550:PHE:HE1	2.34	0.44
1:A:564:GLU:CD	1:A:564:GLU:H	2.21	0.44
1:A:431:LYS:NZ	1:A:431:LYS:HB3	2.33	0.43
1:B:480:LEU:HD12	1:B:480:LEU:HA	1.83	0.43
1:B:30:TYR:O	1:B:31:LEU:HD23	2.17	0.43
1:B:385:ASN:O	1:B:389:GLN:HG3	2.18	0.43
1:B:207:GLU:O	1:B:210:LEU:HB3	2.18	0.43
1:A:326:LEU:HA	1:A:326:LEU:HD23	1.84	0.43
1:B:340:TYR:OH	1:B:380:VAL:HG21	2.18	0.43
1:B:229:GLU:OE2	1:B:229:GLU:CA	2.65	0.43
2:B:602:NPS:H102	2:B:603:NPS:H121	2.01	0.43
1:B:111:ASP:HB2	5:B:727:HOH:O	2.17	0.43
1:B:111:ASP:CG	1:B:111:ASP:O	2.57	0.43
1:B:440:PRO:O	1:B:443:GLU:N	2.52	0.43
1:B:539:THR:O	1:B:540:GLU:C	2.57	0.43
1:B:389:GLN:O	1:B:393:GLN:HB2	2.19	0.42
1:B:374:ASP:O	1:B:375:LYS:C	2.57	0.42
1:B:387:ILE:N	1:B:387:ILE:HD13	2.34	0.42
1:B:501:PHE:CE2	1:B:503:GLU:HG3	2.53	0.42
1:A:7:ILE:HG22	5:A:728:HOH:O	2.19	0.42
1:B:115:LEU:O	1:B:117:PRO:HD3	2.19	0.42
1:B:312:LYS:HG3	1:B:366:HIS:CD2	2.55	0.42
1:B:83:THR:HB	1:B:84:TYR:CE2	2.55	0.42
1:A:517:ASP:O	1:A:521:GLN:HG3	2.19	0.42
1:A:46:LEU:HA	1:A:46:LEU:HD22	1.74	0.42
1:A:67:HIS:CE1	5:A:744:HOH:O	2.73	0.42
1:A:46:LEU:HD23	1:A:73:GLU:HG3	2.00	0.42
1:B:423:VAL:O	1:B:427:ARG:HG3	2.20	0.42
1:B:553:PHE:CD2	1:B:574:LEU:HD22	2.54	0.42
1:B:182:GLU:HG2	5:B:741:HOH:O	2.19	0.42
1:A:241:HIS:NE2	4:A:605:PEG:H42	2.35	0.42
1:A:348:LEU:HD22	1:A:376:LEU:HB3	2.02	0.42
1:A:375:LYS:HE2	1:A:375:LYS:HB3	1.69	0.42
1:A:419:THR:N	1:A:420:PRO:CD	2.82	0.42
1:A:445:MET:N	1:A:446:PRO:HD2	2.35	0.42
2:A:603:NPS:H103	2:A:603:NPS:H11	1.67	0.42
1:B:274:LEU:O	1:B:275:LYS:C	2.59	0.41
1:B:411:THR:HG22	1:B:411:THR:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:CYS:CB	1:B:177:LEU:CD2	2.98	0.41
1:A:178:LEU:N	1:A:179:PRO:CD	2.83	0.41
1:A:340:TYR:N	1:A:340:TYR:CD1	2.88	0.41
1:B:66:LEU:HD22	1:B:250:LEU:HD12	2.03	0.41
1:B:501:PHE:HE2	1:B:503:GLU:HG3	1.85	0.41
1:B:152:GLU:OE1	1:B:287:HIS:ND1	2.48	0.41
1:A:210:LEU:O	1:A:211:LYS:C	2.59	0.41
1:A:237:LEU:HD11	4:A:605:PEG:H41	2.02	0.41
1:B:342:VAL:HG12	1:B:346:LEU:CD1	2.51	0.41
1:B:415:PRO:O	1:B:533:LYS:HE2	2.21	0.41
1:A:167:CYS:HB3	1:A:177:LEU:CD2	2.51	0.41
1:A:199:CYS:HA	1:A:202:ILE:HD12	2.02	0.41
1:B:409:ARG:HH11	1:B:409:ARG:HD3	1.74	0.41
1:B:445:MET:N	1:B:446:PRO:HD2	2.35	0.41
1:B:118:ASP:O	1:B:122:LEU:HG	2.21	0.41
1:B:352:TYR:O	1:B:356:LEU:HG	2.21	0.41
1:B:508:PHE:CE1	1:B:550:PHE:CE1	3.09	0.41
1:A:511:ASP:O	1:A:514:THR:HB	2.21	0.40
1:B:46:LEU:HA	1:B:46:LEU:HD22	1.81	0.40
1:B:155:TYR:HE1	1:B:284:GLU:HG2	1.85	0.40
1:B:330:LEU:HA	1:B:330:LEU:HD12	1.92	0.40
1:B:528:LEU:O	1:B:531:LEU:HB3	2.20	0.40
1:A:85:GLY:O	1:A:87:MET:N	2.55	0.40
1:B:166:GLU:O	1:B:166:GLU:HG2	2.21	0.40
2:B:603:NPS:H11	2:B:603:NPS:H103	1.64	0.40
1:A:66:LEU:O	1:A:70:PHE:HD2	2.04	0.40
1:A:77:VAL:HB	1:A:80:LEU:HD13	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	580/583 (100%)	545 (94%)	33 (6%)	2 (0%)	41	62
1	B	580/583 (100%)	541 (93%)	38 (7%)	1 (0%)	47	69
All	All	1160/1166 (100%)	1086 (94%)	71 (6%)	3 (0%)	41	62

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	86	ASP
1	A	265	ASP
1	B	302	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	520/521 (100%)	477 (92%)	43 (8%)	11	21
1	B	520/521 (100%)	461 (89%)	59 (11%)	6	10
All	All	1040/1042 (100%)	938 (90%)	102 (10%)	8	14

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	3	HIS
1	A	17	GLU
1	A	46	LEU
1	A	76	LYS
1	A	87	MET
1	A	92	GLU
1	A	100	GLU
1	A	116	LYS
1	A	118	ASP
1	A	121	THR
1	A	127	LYS
1	A	130	GLU

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Mol	Chain	Res	Type
1	A	131	LYS
1	A	171	GLU
1	A	173	LYS
1	A	181	ILE
1	A	184	MET
1	A	202	ILE
1	A	208	ARG
1	A	217	ARG
1	A	244	CYS
1	A	268	ASP
1	A	272	SER
1	A	292	VAL
1	A	297	ILE
1	A	299	GLU
1	A	305	THR
1	A	316	LYS
1	A	319	GLN
1	A	385	ASN
1	A	407	ILE
1	A	409	ARG
1	A	413	LYS
1	A	438	THR
1	A	464	GLU
1	A	466	THR
1	A	481	VAL
1	A	488	SER
1	A	495	THR
1	A	514	THR
1	A	544	LYS
1	A	561	ASP
1	B	2	THR
1	B	17	GLU
1	B	30	TYR
1	B	46	LEU
1	B	76	LYS
1	B	79	SER
1	B	83	THR
1	B	86	ASP
1	B	87	MET
1	B	92	GLU
1	B	111	ASP
1	B	116	LYS

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Mol	Chain	Res	Type
1	B	121	THR
1	B	122	LEU
1	B	127	LYS
1	B	130	GLU
1	B	131	LYS
1	B	173	LYS
1	B	181	ILE
1	B	201	SER
1	B	202	ILE
1	B	208	ARG
1	B	217	ARG
1	B	221	LYS
1	B	224	LYS
1	B	235	THR
1	B	244	CYS
1	B	266	ASN
1	B	268	ASP
1	B	282	LEU
1	B	286	SER
1	B	294	LYS
1	B	297	ILE
1	B	311	ASP
1	B	316	LYS
1	B	333	TYR
1	B	343	SER
1	B	350	LYS
1	B	368	CYS
1	B	369	TYR
1	B	375	LYS
1	B	385	ASN
1	B	396	LYS
1	B	409	ARG
1	B	434	THR
1	B	435	ARG
1	B	438	THR
1	B	442	SER
1	B	464	GLU
1	B	466	THR
1	B	481	VAL
1	B	491	THR
1	B	493	ASP
1	B	494	GLU

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Mol	Chain	Res	Type
1	B	495	THR
1	B	513	CYS
1	B	514	THR
1	B	518	THR
1	B	561	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	319	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

8 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	NPS	B	603	-	15,18,18	1.48	4 (26%)	21,25,25	1.92	7 (33%)
2	NPS	A	603	-	15,18,18	1.72	3 (20%)	21,25,25	2.09	10 (47%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PGE	A	604	-	9,9,9	0.53	0	8,8,8	1.38	1 (12%)
4	PEG	A	605	-	6,6,6	0.43	0	5,5,5	1.55	1 (20%)
2	NPS	B	602	-	15,18,18	1.37	4 (26%)	21,25,25	1.39	4 (19%)
2	NPS	B	601	-	15,18,18	1.51	2 (13%)	21,25,25	1.41	3 (14%)
2	NPS	A	601	-	15,18,18	1.25	2 (13%)	21,25,25	1.49	5 (23%)
2	NPS	A	602	-	15,18,18	1.16	1 (6%)	21,25,25	1.49	3 (14%)

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	NPS	B	603	-	-	2/6/10/10	0/2/2/2
2	NPS	A	603	-	-	2/6/10/10	0/2/2/2
3	PGE	A	604	-	-	4/7/7/7	-
4	PEG	A	605	-	-	3/4/4/4	-
2	NPS	B	602	-	-	2/6/10/10	0/2/2/2
2	NPS	B	601	-	-	0/6/10/10	0/2/2/2
2	NPS	A	601	-	-	0/6/10/10	0/2/2/2
2	NPS	A	602	-	-	2/6/10/10	0/2/2/2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	603	NPS	C8-C14	-3.14	1.47	1.52
2	A	603	NPS	C6-C1	2.89	1.42	1.37
2	B	601	NPS	C6-C1	2.83	1.42	1.37
2	A	601	NPS	C10-C14	-2.53	1.48	1.53
2	A	602	NPS	C6-C1	2.48	1.41	1.37
2	B	603	NPS	C8-C14	-2.43	1.48	1.52
2	A	603	NPS	C10-C14	-2.39	1.49	1.53
2	B	603	NPS	C3-C2	2.34	1.41	1.36
2	B	602	NPS	C11-C8	2.33	1.42	1.39
2	B	602	NPS	C6-C1	2.28	1.41	1.37
2	B	601	NPS	C8-C14	-2.28	1.48	1.52
2	B	602	NPS	C13-C11	2.26	1.41	1.36
2	B	603	NPS	C7-C8	2.26	1.41	1.37
2	A	601	NPS	C2-C1	2.25	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	603	NPS	C2-C1	2.21	1.43	1.38
2	B	602	NPS	C10-C14	-2.20	1.49	1.53

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	603	NPS	C6-C5-C4	3.76	124.32	118.96
2	A	603	NPS	C8-C7-C4	-3.68	115.99	121.48
2	B	603	NPS	C6-C5-C4	3.64	124.16	118.96
2	B	603	NPS	C11-C8-C14	-3.44	113.85	120.96
2	A	602	NPS	C7-C4-C5	3.23	123.57	118.96
2	B	603	NPS	C8-C7-C4	-3.19	116.72	121.48
2	B	602	NPS	C10-C14-C15	-3.17	103.94	112.14
2	B	603	NPS	C13-C5-C6	-3.14	116.48	122.02
2	A	603	NPS	C13-C5-C6	-3.04	116.65	122.02
2	B	601	NPS	C3-C4-C7	-3.00	116.73	122.02
2	B	601	NPS	C7-C8-C14	-2.97	115.45	122.20
2	A	603	NPS	C1-C6-C5	-2.93	115.47	119.70
2	B	602	NPS	C7-C4-C5	2.82	122.99	118.96
2	A	603	NPS	C7-C4-C5	2.78	122.93	118.96
2	A	601	NPS	C1-C6-C5	-2.64	115.90	119.70
2	A	601	NPS	C10-C14-C15	-2.63	105.33	112.14
2	A	602	NPS	C3-C4-C7	-2.46	117.67	122.02
2	B	602	NPS	C3-C4-C7	-2.46	117.67	122.02
2	A	601	NPS	C6-C5-C4	2.42	122.41	118.96
2	B	603	NPS	C1-C6-C5	-2.40	116.25	119.70
2	A	603	NPS	C3-C4-C7	-2.35	117.88	122.02
2	B	603	NPS	C10-C14-C15	-2.28	106.24	112.14
2	A	603	NPS	C10-C14-C15	-2.25	106.30	112.14
2	A	601	NPS	C13-C5-C6	-2.25	118.05	122.02
2	A	603	NPS	C2-C3-C4	-2.23	117.37	120.82
2	B	603	NPS	C11-C8-C7	2.20	121.43	118.60
2	A	603	NPS	C11-C8-C14	-2.19	116.43	120.96
2	B	601	NPS	C11-C8-C7	2.19	121.42	118.60
2	A	603	NPS	C3-C2-C1	2.14	123.05	120.17
3	A	604	PGE	O3-C4-C3	2.13	119.99	110.39
4	A	605	PEG	C3-O2-C2	2.12	122.49	113.29
2	A	602	NPS	C6-C5-C4	2.11	121.97	118.96
2	A	601	NPS	O2-C1-C6	-2.10	118.70	124.43
2	B	602	NPS	C8-C7-C4	-2.09	118.37	121.48

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	603	NPS	C6-C1-O2-C12
2	B	602	NPS	C2-C1-O2-C12
2	B	603	NPS	C2-C1-O2-C12
2	B	602	NPS	C6-C1-O2-C12
4	A	605	PEG	C4-C3-O2-C2
2	A	602	NPS	C6-C1-O2-C12
3	A	604	PGE	O2-C3-C4-O3
2	A	603	NPS	C6-C1-O2-C12
4	A	605	PEG	O1-C1-C2-O2
4	A	605	PEG	O2-C3-C4-O4
2	A	603	NPS	C2-C1-O2-C12
2	A	602	NPS	C2-C1-O2-C12
3	A	604	PGE	O3-C5-C6-O4
3	A	604	PGE	O1-C1-C2-O2
3	A	604	PGE	C6-C5-O3-C4

There are no ring outliers.

6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	603	NPS	3	0
2	A	603	NPS	1	0
4	A	605	PEG	2	0
2	B	602	NPS	3	0
2	B	601	NPS	1	0
2	A	601	NPS	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

6.1 Protein, DNA and RNA chains

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	582/583 (99%)	-0.21	12 (2%) 63 60	33, 59, 105, 139	0
1	B	582/583 (99%)	-0.15	11 (1%) 66 64	40, 68, 112, 136	0
All	All	1164/1166 (99%)	-0.18	23 (1%) 65 62	33, 64, 110, 139	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	THR	5.2
1	A	3	HIS	3.9
1	A	128	ALA	3.6
1	B	2	THR	3.6
1	A	170	ALA	3.3
1	A	83	THR	2.9
1	A	172	ASP	2.8
1	B	83	THR	2.7
1	B	82	GLU	2.7
1	B	3	HIS	2.6
1	B	364	ASP	2.6
1	A	330	LEU	2.5
1	A	30	TYR	2.4
1	B	124	ASP	2.4
1	A	171	GLU	2.4
1	A	28	SER	2.4
1	A	26	ALA	2.3
1	B	320	GLU	2.2
1	A	216	ALA	2.1
1	B	119	PRO	2.1
1	B	359	CYS	2.1
1	B	370	SER	2.0
1	B	378	HIS	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(\AA^2)	Q<0.9
4	PEG	A	605	7/7	0.89	0.41	59,74,82,90	0
2	NPS	B	602	17/17	0.90	0.19	71,82,91,97	0
2	NPS	A	603	17/17	0.93	0.19	56,71,85,105	0
3	PGE	A	604	10/10	0.93	0.33	59,73,85,88	0
2	NPS	A	602	17/17	0.94	0.16	62,71,83,84	0
2	NPS	B	603	17/17	0.95	0.15	55,69,104,106	0
2	NPS	A	601	17/17	0.96	0.24	50,57,79,81	0
2	NPS	B	601	17/17	0.96	0.22	57,70,94,99	0

6.5 Other polymers [i](#)

There are no such residues in this entry.