



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 02:17 PM UTC

PDB ID : 4F5V / pdb_00004f5v
Title : Crystal Structure of Leporine Serum Albumin
Authors : Bujacz, A.; Bujacz, G.
Deposited on : 2012-05-13
Resolution : 2.27 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

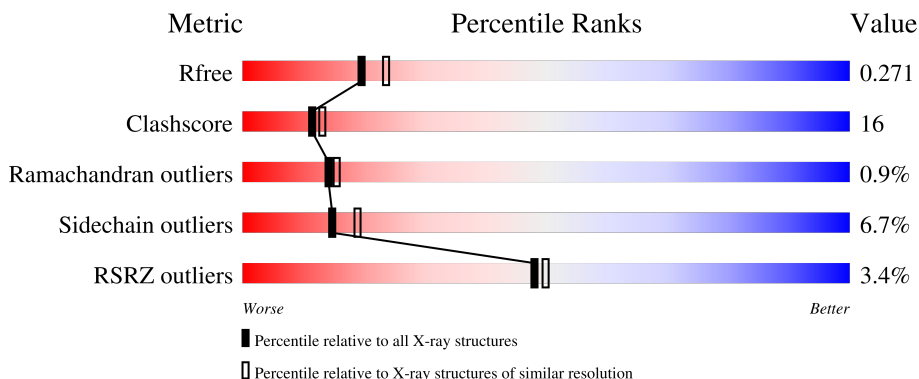
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.27 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	584	 3% 68% 28% . .

2 Entry composition [i](#)

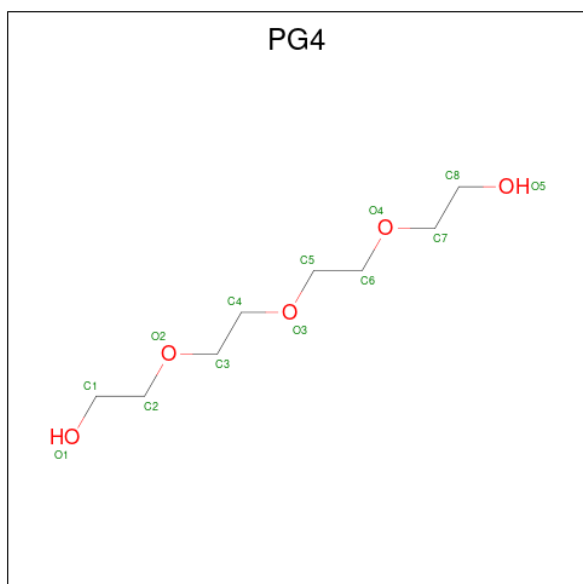
There are 5 unique types of molecules in this entry. The entry contains 4887 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	A	584	4653	2944	781	892	36	0	4	0

- Molecule 2 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



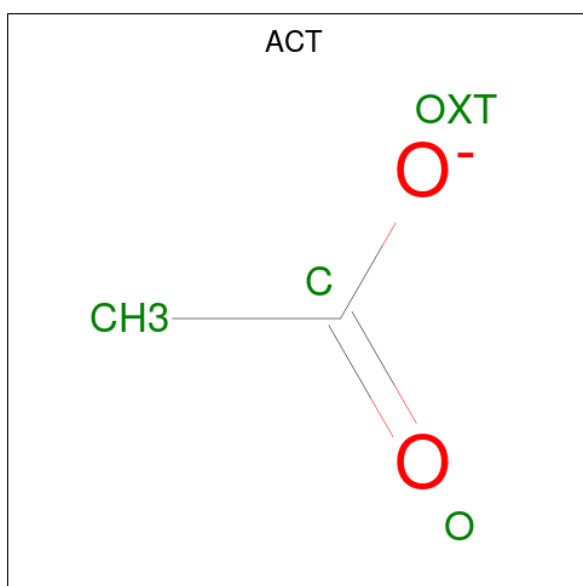
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	13	8	5	0	0

- Molecule 3 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



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

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2^-$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	193	Total 193	O 193	0	0

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: Serum albumin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.20Å 79.64Å 104.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.27 50.00 – 2.27	Depositor EDS
% Data completeness (in resolution range)	93.0 (50.00-2.27) 93.0 (50.00-2.27)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.76 (at 2.27Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.193 , 0.258 0.210 , 0.271	Depositor DCC
R_{free} test set	1478 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	46.8	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 48.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4887	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% 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: ACT, PGE, PG4

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	1.17	7/4766 (0.1%)	1.28	21/6444 (0.3%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	467	THR	CA-CB	8.38	1.62	1.53
1	A	261	ALA	CA-CB	6.20	1.62	1.53
1	A	469	VAL	CA-CB	5.93	1.62	1.54
1	A	334	TYR	CA-C	5.74	1.60	1.52
1	A	425	GLU	CA-C	5.41	1.59	1.52
1	A	344	VAL	CA-CB	5.25	1.61	1.54
1	A	189	ALA	CA-CB	5.01	1.61	1.53

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	481	LEU	N-CA-C	-8.46	99.85	112.04
1	A	300	ALA	N-CA-C	7.04	119.85	111.33
1	A	242	HIS	N-CA-C	6.77	118.66	111.28
1	A	14	VAL	CB-CA-C	6.76	118.25	110.88
1	A	281	LYS	N-CA-C	6.56	119.15	110.36
1	A	34	CYS	N-CA-C	6.37	117.73	109.64
1	A	373	VAL	N-CA-C	6.29	116.78	110.23
1	A	512	ASP	N-CA-C	-6.25	104.47	111.28
1	A	510	HIS	N-CA-C	-6.13	97.75	110.80
1	A	302	LEU	N-CA-C	6.12	117.52	109.93
1	A	467	THR	CB-CA-C	-5.72	102.21	111.14
1	A	168	CYS	N-CA-C	5.63	117.09	111.07
1	A	344	VAL	CB-CA-C	5.37	119.63	112.22
1	A	434	GLY	N-CA-C	5.34	119.10	112.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	397	GLN	N-CA-C	5.29	116.73	111.07
1	A	89	ASP	N-CA-C	-5.21	106.18	112.54
1	A	81	ARG	N-CA-C	5.18	121.84	110.80
1	A	278	CYS	N-CA-C	5.14	117.55	111.33
1	A	527	THR	N-CA-C	-5.10	105.80	111.36
1	A	18	HIS	N-CA-C	-5.04	105.98	111.82
1	A	338	HIS	N-CA-C	5.03	118.27	108.21

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	4653	0	4556	150	0
2	A	13	0	18	0	0
3	A	20	0	28	7	0
4	A	8	0	6	0	0
5	A	193	0	0	33	0
All	All	4887	0	4608	150	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 16.

All (150) 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:582:THR:HB	5:A:892:HOH:O	1.51	1.08
1:A:471[B]:GLU:HG3	5:A:857:HOH:O	1.63	0.97
1:A:235:VAL:O	1:A:239:THR:HG23	1.67	0.94
1:A:386:ASN:HB3	5:A:794:HOH:O	1.67	0.93
1:A:32:GLN:HE22	1:A:107:ASP:H	1.16	0.89
1:A:410:ARG:HH11	3:A:603:PGE:C5	1.88	0.86
1:A:512:ASP:HB2	5:A:893:HOH:O	1.76	0.86
1:A:212:LYS:HG2	1:A:239:THR:HG21	1.58	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:THR:HA	5:A:828:HOH:O	1.78	0.83
1:A:471[B]:GLU:H	1:A:471[B]:GLU:CD	1.87	0.81
1:A:507:PHE:HZ	1:A:531:GLU:HG3	1.47	0.80
1:A:87:VAL:HA	1:A:89:ASP:OD2	1.83	0.79
1:A:316:CYS:O	1:A:320:GLU:HG3	1.85	0.77
1:A:82:ASP:HB3	5:A:874:HOH:O	1.87	0.74
1:A:507:PHE:HD2	5:A:873:HOH:O	1.71	0.73
1:A:33:LYS:HE2	1:A:85:GLY:HA2	1.70	0.72
1:A:3:HIS:NE2	5:A:764:HOH:O	2.24	0.70
1:A:32:GLN:HE22	1:A:107:ASP:N	1.89	0.70
1:A:351:LYS:HE3	5:A:759:HOH:O	1.91	0.70
1:A:466:LYS:NZ	5:A:769:HOH:O	2.27	0.68
1:A:84:TYR:HD1	1:A:85:GLY:N	1.92	0.68
1:A:81:ARG:HE	1:A:82:ASP:H	1.42	0.67
1:A:391:ASN:HD21	1:A:410:ARG:HH12	1.42	0.67
1:A:458:ASN:HD22	1:A:484:ARG:HH12	1.43	0.66
1:A:283:ILE:HG13	5:A:877:HOH:O	1.96	0.66
1:A:74:ILE:O	1:A:77:LEU:HB3	1.96	0.65
1:A:245:CYS:SG	5:A:718:HOH:O	2.55	0.65
1:A:283:ILE:CG1	5:A:877:HOH:O	2.45	0.65
1:A:194:ALA:HB1	1:A:455:VAL:HG13	1.80	0.64
1:A:410:ARG:HH11	3:A:603:PGE:H52	1.61	0.64
1:A:500:LYS:HA	5:A:849:HOH:O	1.95	0.64
1:A:507:PHE:CD1	5:A:858:HOH:O	2.50	0.64
1:A:410:ARG:NH1	3:A:603:PGE:H52	2.12	0.63
1:A:59:ALA:HB3	1:A:62:CYS:SG	2.38	0.63
1:A:480:SER:HB3	1:A:483:ASP:H	1.64	0.63
1:A:410:ARG:NH1	3:A:603:PGE:C5	2.61	0.62
1:A:84:TYR:CD1	1:A:85:GLY:N	2.67	0.62
1:A:32:GLN:NE2	1:A:107:ASP:H	1.94	0.62
1:A:77:LEU:C	1:A:79:SER:N	2.59	0.61
1:A:410:ARG:HH11	3:A:603:PGE:H5	1.63	0.60
1:A:294:HIS:HD2	5:A:842:HOH:O	1.85	0.59
1:A:580:LYS:O	1:A:584:GLY:HA2	2.02	0.59
1:A:39:HIS:O	1:A:43:VAL:HG23	2.03	0.58
1:A:77:LEU:C	1:A:79:SER:H	2.10	0.58
1:A:512:ASP:O	1:A:515:THR:HG22	2.03	0.58
1:A:77:LEU:H	1:A:78:PRO:HD2	1.69	0.57
1:A:225:LYS:HE2	1:A:296:ASP:OD2	2.03	0.57
1:A:356:THR:CA	5:A:828:HOH:O	2.46	0.57
1:A:29:GLN:HG2	1:A:147:PRO:HA	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:ARG:NE	5:A:826:HOH:O	2.37	0.57
1:A:42:LEU:CD2	1:A:73:LYS:HB3	2.35	0.56
1:A:74:ILE:O	1:A:77:LEU:CB	2.54	0.56
1:A:480:SER:HB2	5:A:705:HOH:O	2.05	0.56
1:A:580:LYS:O	1:A:584:GLY:CA	2.54	0.55
1:A:304:ALA:HB3	1:A:307:GLU:HG3	1.89	0.55
1:A:33:LYS:CE	1:A:85:GLY:HA2	2.37	0.55
1:A:45:GLU:HB3	1:A:73:LYS:HE3	1.89	0.54
1:A:507:PHE:HB2	1:A:551:PHE:HE1	1.72	0.54
1:A:179:THR:OG1	1:A:180:PRO:HD3	2.07	0.54
1:A:141:GLU:OE1	1:A:145:ARG:NH1	2.28	0.53
1:A:408:LEU:HD21	1:A:424:VAL:HA	1.90	0.53
1:A:117:ARG:HG2	1:A:118:PRO:O	2.09	0.53
1:A:433:VAL:HG22	1:A:452:TYR:CG	2.44	0.53
1:A:240:LYS:HE3	5:A:817:HOH:O	2.10	0.52
1:A:37:GLU:OE1	1:A:37:GLU:N	2.38	0.52
1:A:507:PHE:CZ	1:A:531:GLU:HG3	2.37	0.52
1:A:77:LEU:N	1:A:78:PRO:HD2	2.24	0.52
1:A:93:LYS:HE3	1:A:97:GLU:HB3	1.92	0.52
1:A:104:HIS:HB3	5:A:838:HOH:O	2.09	0.52
1:A:84:TYR:HD1	1:A:84:TYR:C	2.19	0.51
1:A:47:THR:HG22	1:A:51:LYS:HE3	1.93	0.51
1:A:84:TYR:CD1	1:A:84:TYR:C	2.89	0.51
1:A:380:LEU:O	1:A:384:PRO:HD2	2.10	0.51
1:A:125:LYS:NZ	1:A:129:ASP:OD1	2.40	0.51
1:A:33:LYS:HD2	1:A:84:TYR:CD1	2.46	0.50
1:A:341:TYR:HA	1:A:446:LEU:HD23	1.92	0.50
1:A:355:ALA:C	5:A:828:HOH:O	2.54	0.50
1:A:16:GLU:O	1:A:20:ILE:HG13	2.12	0.50
1:A:378:GLN:HE21	1:A:382:ASP:CG	2.19	0.50
1:A:507:PHE:CD2	5:A:873:HOH:O	2.53	0.50
1:A:305:VAL:HG13	1:A:374:LEU:HD13	1.94	0.49
1:A:240:LYS:CE	5:A:817:HOH:O	2.61	0.48
1:A:373:VAL:HG13	1:A:374:LEU:N	2.28	0.48
1:A:390:GLN:HG3	5:A:878:HOH:O	2.13	0.48
1:A:505:GLU:HG2	1:A:572:GLY:C	2.38	0.48
1:A:47:THR:O	1:A:51:LYS:HG2	2.13	0.48
1:A:378:GLN:NE2	1:A:382:ASP:OD1	2.46	0.48
1:A:412:THR:O	1:A:416:PRO:HB3	2.14	0.47
1:A:436:LYS:NZ	5:A:756:HOH:O	2.41	0.47
1:A:443:ALA:C	5:A:754:HOH:O	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:ARG:CG	1:A:482:VAL:HG12	2.44	0.47
1:A:14:VAL:HG12	1:A:19:PHE:HB2	1.96	0.47
1:A:38:GLU:OE1	1:A:80:LEU:HD13	2.14	0.46
1:A:279:CYS:HA	1:A:286:LYS:HD2	1.97	0.46
1:A:545:LYS:NZ	3:A:602:PGE:H6	2.30	0.46
1:A:182:LEU:HD12	1:A:182:LEU:HA	1.80	0.46
1:A:135:PHE:CZ	1:A:162:LYS:HB2	2.51	0.46
1:A:194:ALA:CB	1:A:455:VAL:HG13	2.45	0.46
1:A:348:ARG:HG3	1:A:482:VAL:CG1	2.46	0.46
1:A:446:LEU:HB3	1:A:447:PRO:HD3	1.97	0.46
1:A:408:LEU:HD22	1:A:530:VAL:HG23	1.97	0.45
1:A:294:HIS:CD2	1:A:294:HIS:H	2.32	0.45
1:A:580:LYS:O	1:A:584:GLY:N	2.50	0.45
1:A:344:VAL:HG22	1:A:482:VAL:HG13	1.98	0.45
1:A:120:ALA:HB1	1:A:174:LYS:HB2	1.99	0.45
1:A:223:PHE:HD1	1:A:272:SER:HB2	1.80	0.45
1:A:114:PRO:O	1:A:116:ALA:N	2.50	0.45
1:A:277[B]:GLU:OE1	1:A:281:LYS:HE2	2.17	0.45
1:A:408:LEU:HD22	1:A:530:VAL:CG2	2.47	0.44
1:A:372:LYS:C	5:A:729:HOH:O	2.60	0.44
1:A:405:ASN:HB3	3:A:602:PGE:H4	2.00	0.44
1:A:472:LYS:HD3	1:A:491:LEU:HD22	1.99	0.44
1:A:120:ALA:CB	1:A:174:LYS:HB2	2.47	0.44
1:A:298:THR:HG22	1:A:336:ARG:O	2.18	0.44
1:A:378:GLN:N	1:A:379:PRO:CD	2.80	0.44
1:A:378:GLN:N	1:A:379:PRO:HD2	2.32	0.44
1:A:532:LEU:HD11	1:A:547:VAL:HG12	2.00	0.44
1:A:240:LYS:NZ	5:A:817:HOH:O	2.36	0.43
1:A:249:ASP:HB3	1:A:252:GLU:HG2	1.99	0.43
1:A:554:LEU:HD12	1:A:571:GLU:HB3	2.00	0.43
1:A:161:TYR:CE1	1:A:165:LEU:HD11	2.53	0.43
1:A:545:LYS:HE3	1:A:545:LYS:HB2	1.41	0.43
1:A:249:ASP:HB3	1:A:252:GLU:CG	2.48	0.43
1:A:49:LEU:O	1:A:49:LEU:HG	2.18	0.43
1:A:50:ALA:O	1:A:54:VAL:HG23	2.19	0.43
1:A:121:ASP:OD1	1:A:174:LYS:HE2	2.19	0.42
1:A:283:ILE:HG12	5:A:877:HOH:O	2.13	0.42
1:A:373:VAL:HG13	1:A:374:LEU:H	1.84	0.42
1:A:377:PHE:C	1:A:379:PRO:HD2	2.44	0.42
1:A:7:ILE:HG22	5:A:744:HOH:O	2.19	0.42
1:A:165:LEU:O	1:A:169:CYS:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:PHE:CD2	1:A:19:PHE:C	2.98	0.42
1:A:35:PRO:HD2	1:A:84:TYR:OH	2.20	0.42
1:A:532:LEU:HD11	1:A:547:VAL:CG1	2.50	0.42
1:A:205:LYS:HD3	1:A:206:PHE:CE2	2.55	0.41
1:A:223:PHE:N	1:A:224:PRO:CD	2.82	0.41
1:A:316:CYS:HB2	5:A:727:HOH:O	2.20	0.41
1:A:482:VAL:HG12	1:A:482:VAL:O	2.20	0.41
1:A:131:GLU:OE1	1:A:162:LYS:HE2	2.21	0.41
1:A:152:PRO:HB2	1:A:257:ARG:HH11	1.85	0.41
1:A:356:THR:N	5:A:828:HOH:O	2.54	0.41
1:A:509:PHE:CD2	1:A:513:ILE:HD11	2.56	0.41
1:A:77:LEU:N	1:A:78:PRO:CD	2.84	0.40
1:A:118:PRO:HG2	1:A:123:LEU:HD13	2.03	0.40
1:A:211:TYR:CD2	1:A:239:THR:HG22	2.56	0.40
1:A:348:ARG:HH22	1:A:450:GLU:CD	2.29	0.40
1:A:525:LYS:HE2	1:A:552:THR:HB	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	586/584 (100%)	540 (92%)	41 (7%)	5 (1%)	14 15

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	115	PHE
1	A	504	ALA
1	A	81	ARG
1	A	78	PRO
1	A	513	ILE

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	514/510 (101%)	479 (93%)	35 (7%)	14	18

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	HIS
1	A	14	VAL
1	A	84	TYR
1	A	89	ASP
1	A	173	ASP
1	A	243	LYS
1	A	245	CYS
1	A	283	ILE
1	A	286	LYS
1	A	311	GLU
1	A	343	VAL
1	A	344	VAL
1	A	372	LYS
1	A	426	ILE
1	A	435	SER
1	A	436	LYS
1	A	455	VAL
1	A	462	VAL
1	A	466	LYS
1	A	469	VAL
1	A	471[A]	GLU
1	A	471[B]	GLU
1	A	475	LYS
1	A	480	SER
1	A	481	LEU
1	A	496	THR
1	A	500	LYS
1	A	505	GLU
1	A	510	HIS
1	A	512	ASP

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Mol	Chain	Res	Type
1	A	513	ILE
1	A	552	THR
1	A	565	GLU
1	A	582	THR
1	A	583	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	29	GLN
1	A	32	GLN
1	A	268	GLN
1	A	294	HIS
1	A	318	ASN
1	A	378	GLN
1	A	386	ASN
1	A	390	GLN
1	A	391	ASN
1	A	458	ASN
1	A	510	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 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	$\# Z > 2$
3	PGE	A	603	-	9,9,9	0.47	0	8,8,8	1.47	2 (25%)
4	ACT	A	604	-	3,3,3	0.79	0	3,3,3	1.63	1 (33%)
4	ACT	A	605	-	3,3,3	0.74	0	3,3,3	1.61	1 (33%)
2	PG4	A	601	-	12,12,12	0.84	0	11,11,11	0.77	0
3	PGE	A	602	-	9,9,9	0.75	0	8,8,8	0.63	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
3	PGE	A	603	-	-	4/7/7/7	-
3	PGE	A	602	-	-	3/7/7/7	-
2	PG4	A	601	-	-	5/10/10/10	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	603	PGE	O4-C6-C5	-2.36	97.91	111.82
4	A	604	ACT	OXT-C-O	-2.25	113.67	122.03
3	A	603	PGE	O3-C5-C6	-2.16	100.60	110.11
4	A	605	ACT	OXT-C-CH3	2.02	123.50	115.05

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	PG4	O3-C5-C6-O4
3	A	603	PGE	O3-C5-C6-O4
3	A	602	PGE	O2-C3-C4-O3

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Mol	Chain	Res	Type	Atoms
2	A	601	PG4	O4-C7-C8-O5
3	A	602	PGE	O3-C5-C6-O4
2	A	601	PG4	C1-C2-O2-C3
3	A	603	PGE	C6-C5-O3-C4
3	A	603	PGE	O1-C1-C2-O2
3	A	602	PGE	C6-C5-O3-C4
3	A	603	PGE	O2-C3-C4-O3
2	A	601	PG4	C4-C3-O2-C2
2	A	601	PG4	O2-C3-C4-O3

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	603	PGE	5	0
3	A	602	PGE	2	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	584/584 (100%)	0.20	20 (3%)	48 50	28, 54, 110, 158	4 (0%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	502	PHE	3.7
1	A	102	PHE	3.3
1	A	176	ALA	3.2
1	A	555	LEU	3.2
1	A	2	ALA	3.1
1	A	510	HIS	3.1
1	A	77	LEU	2.8
1	A	507	PHE	2.6
1	A	511	ALA	2.6
1	A	87	VAL	2.5
1	A	503	ASN	2.4
1	A	509	PHE	2.4
1	A	535	HIS	2.4
1	A	567	CYS	2.3
1	A	78	PRO	2.3
1	A	506	THR	2.3
1	A	513	ILE	2.3
1	A	96	PRO	2.1
1	A	551	PHE	2.1
1	A	83	THR	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PG4	A	601	13/13	0.83	0.16	58,66,70,72	0
3	PGE	A	602	10/10	0.85	0.14	59,63,67,70	0
3	PGE	A	603	10/10	0.88	0.10	46,51,57,57	0
4	ACT	A	605	4/4	0.94	0.12	51,51,51,52	0
4	ACT	A	604	4/4	0.96	0.08	43,45,45,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.