



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:45 AM UTC

PDB ID : 4PO0 / pdb_00004po0
Title : Crystal Structure of Leporine Serum Albumin in complex with naproxen
Authors : Zielinski, K.; Bujacz, A.; Sekula, B.; Bujacz, G.
Deposited on : 2014-02-23
Resolution : 2.73 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

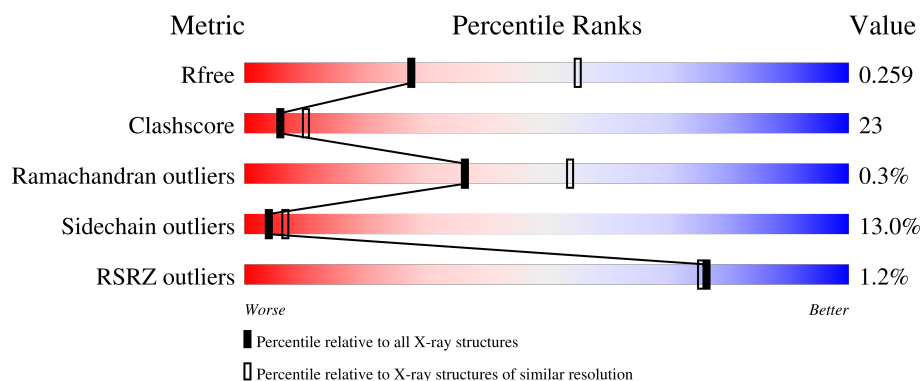
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.73 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	1819 (2.76-2.72)
Clashscore	190562	1866 (2.76-2.72)
Ramachandran outliers	187476	1830 (2.76-2.72)
Sidechain outliers	187428	1831 (2.76-2.72)
RSRZ outliers	180081	1819 (2.76-2.72)

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	

2 Entry composition [i](#)

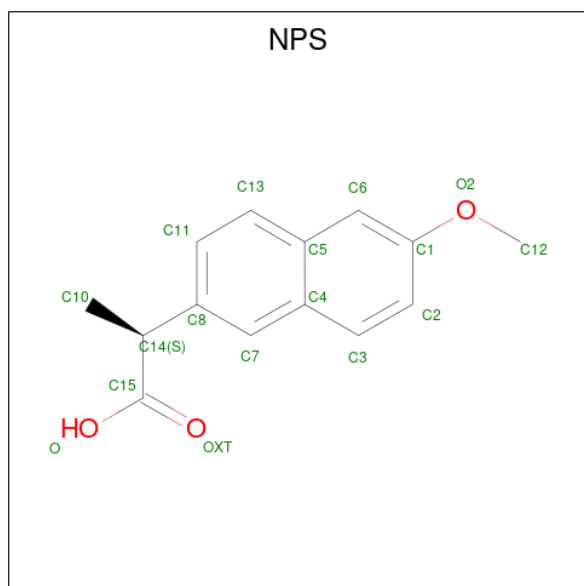
There are 3 unique types of molecules in this entry. The entry contains 4813 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	583	4641	2937	782	886	36	0	3	0

- Molecule 2 is (2S)-2-(6-methoxynaphthalen-2-yl)propanoic acid (CCD ID: NPS) (formula: C₁₄H₁₄O₃).



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

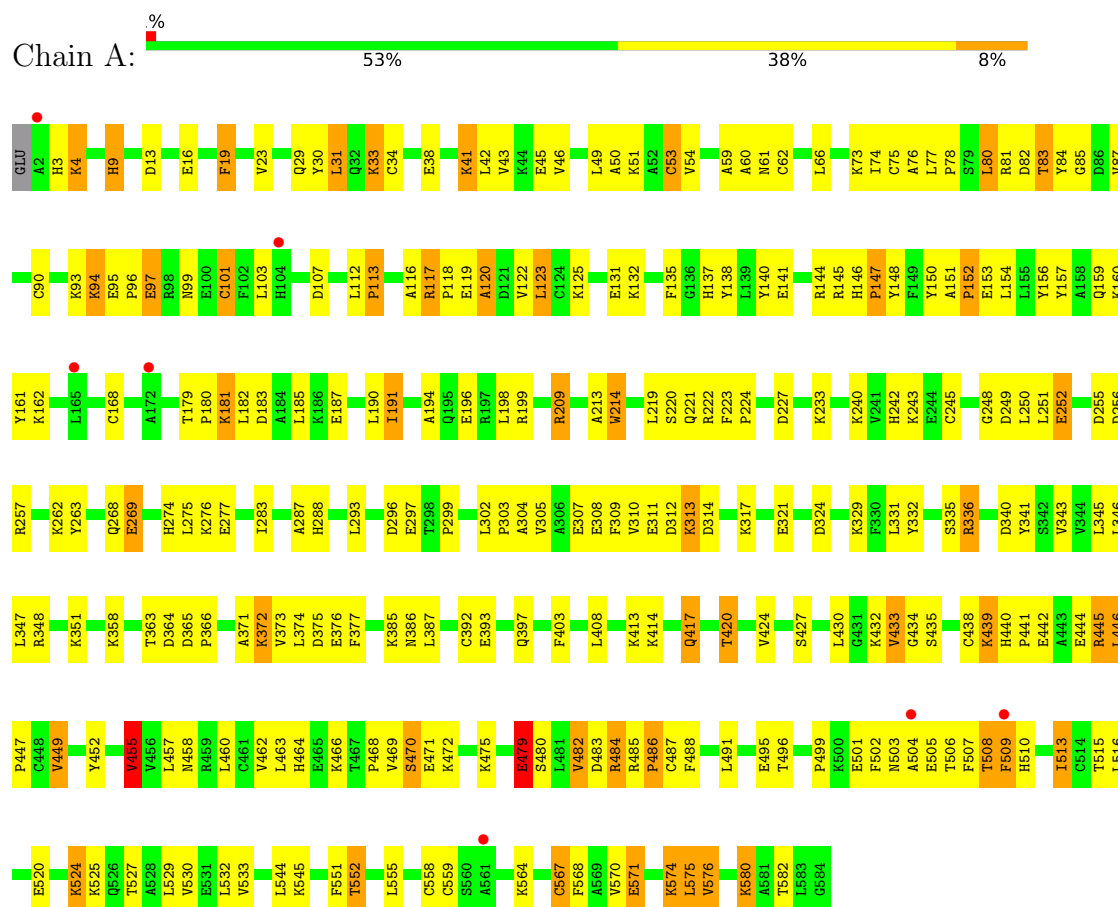
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	121	Total 121	O 121	0	0

3 Residue-property plots

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	74.44Å 79.79Å 102.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.11 – 2.73 48.11 – 2.73	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.11-2.73) 99.8 (48.11-2.73)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.186 , 0.259 0.186 , 0.259	Depositor DCC
R_{free} test set	843 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	54.7	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 55.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4813	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.28% 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: 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	1.08	2/4752 (0.0%)	1.37	36/6424 (0.6%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	420	THR	N-CA	-6.20	1.40	1.46
1	A	463	LEU	N-CA	5.68	1.53	1.46

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	283	ILE	N-CA-C	8.90	119.70	110.36
1	A	509	PHE	N-CA-C	8.64	119.64	108.24
1	A	433	VAL	CB-CA-C	-7.89	101.49	112.14
1	A	403	PHE	N-CA-C	-7.63	103.04	111.36
1	A	420	THR	CA-C-N	-7.51	111.23	119.19
1	A	420	THR	C-N-CA	-7.51	111.23	119.19
1	A	9	HIS	N-CA-C	-7.14	103.43	111.07
1	A	256	ASP	N-CA-C	-6.94	103.77	111.82
1	A	479	GLU	N-CA-C	6.80	118.77	111.36
1	A	220	SER	N-CA-C	-6.70	103.22	111.40
1	A	268	GLN	N-CA-C	6.60	119.32	111.33
1	A	570	VAL	N-CA-C	6.60	117.22	110.82
1	A	445	ARG	N-CA-C	6.41	118.06	111.14
1	A	576	VAL	N-CA-C	-6.29	104.20	110.30
1	A	446	LEU	CA-C-N	-6.22	112.77	119.24
1	A	446	LEU	C-N-CA	-6.22	112.77	119.24
1	A	113	PRO	CA-C-N	-6.18	113.41	119.78
1	A	113	PRO	C-N-CA	-6.18	113.41	119.78
1	A	358	LYS	N-CA-C	-6.13	104.52	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	53	CYS	N-CA-C	-6.00	103.39	112.04
1	A	179	THR	CA-C-N	-5.91	112.46	119.84
1	A	179	THR	C-N-CA	-5.91	112.46	119.84
1	A	449	VAL	N-CA-C	5.68	115.76	110.42
1	A	455	VAL	N-CA-CB	-5.65	102.10	110.58
1	A	145	ARG	N-CA-C	-5.51	106.60	113.38
1	A	214	TRP	N-CA-C	-5.49	105.31	112.23
1	A	533	VAL	N-CA-C	-5.43	104.95	112.50
1	A	385	LYS	N-CA-C	-5.33	105.37	111.07
1	A	60	ALA	N-CA-C	-5.26	102.69	110.48
1	A	427	SER	N-CA-C	-5.23	105.75	111.82
1	A	76	ALA	N-CA-C	-5.21	106.78	112.72
1	A	499	PRO	N-CA-C	5.19	119.46	111.21
1	A	248	GLY	N-CA-C	5.11	125.29	113.18
1	A	469	VAL	CB-CA-C	-5.10	105.84	110.63
1	A	168	CYS	N-CA-C	5.09	119.54	113.23
1	A	101	CYS	N-CA-C	-5.06	105.22	111.40

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	4641	0	4544	208	0
2	A	51	0	39	11	0
3	A	121	0	0	15	0
All	All	4813	0	4583	212	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 23.

All (212) 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:87:VAL:HG12	1:A:90:CYS:SG	1.77	1.23
1:A:87:VAL:CG1	1:A:90:CYS:SG	2.32	1.17
2:A:602:NPS:H11	3:A:819:HOH:O	1.44	1.15
1:A:194:ALA:HB1	1:A:455:VAL:HG13	1.39	1.03
1:A:580:LYS:HB2	3:A:795:HOH:O	1.56	1.03
1:A:38:GLU:OE2	1:A:80:LEU:HG	1.63	0.95
1:A:363:THR:HG22	1:A:365:ASP:H	1.33	0.93
1:A:372:LYS:NZ	1:A:372:LYS:HB3	1.89	0.87
1:A:23:VAL:HG12	1:A:43:VAL:HG22	1.60	0.84
1:A:516:LEU:HB3	1:A:520:GLU:HB2	1.58	0.84
1:A:442:GLU:HA	1:A:445:ARG:HD2	1.58	0.84
1:A:414:LYS:HE3	1:A:491:LEU:O	1.80	0.81
1:A:233:LYS:HE2	1:A:263:TYR:CZ	2.15	0.81
1:A:214:TRP:NE1	1:A:343:VAL:HG21	1.96	0.81
1:A:505:GLU:OE2	1:A:508:THR:HG21	1.81	0.80
1:A:194:ALA:CB	1:A:455:VAL:HG13	2.11	0.80
1:A:525:LYS:HE2	1:A:552:THR:OG1	1.82	0.79
1:A:430:LEU:O	1:A:433:VAL:HG23	1.81	0.78
1:A:317:LYS:O	1:A:321:GLU:HG3	1.83	0.77
1:A:16:GLU:OE1	1:A:51:LYS:HE3	1.84	0.77
1:A:372:LYS:HB3	1:A:372:LYS:HZ3	1.49	0.74
1:A:87:VAL:HG13	1:A:90:CYS:SG	2.30	0.71
1:A:269:GLU:CD	1:A:269:GLU:H	1.98	0.71
1:A:480:SER:OG	1:A:483:ASP:HB2	1.91	0.71
1:A:116:ALA:HB1	3:A:820:HOH:O	1.91	0.70
1:A:222:ARG:HD3	1:A:293:LEU:HB3	1.72	0.69
1:A:187[A]:GLU:OE2	1:A:432:LYS:NZ	2.26	0.68
1:A:505:GLU:HA	1:A:508:THR:HB	1.75	0.68
1:A:45:GLU:HG3	3:A:734:HOH:O	1.94	0.68
1:A:224:PRO:HB2	1:A:299:PRO:HD3	1.76	0.68
1:A:95:GLU:OE1	1:A:99:ASN:HB2	1.95	0.67
1:A:233:LYS:HE2	1:A:263:TYR:CE2	2.29	0.67
1:A:78:PRO:HG3	1:A:82:ASP:OD1	1.96	0.66
1:A:78:PRO:HA	1:A:82:ASP:OD2	1.95	0.66
1:A:559:CYS:HA	1:A:564:LYS:HD3	1.77	0.66
1:A:156:TYR:OH	1:A:160:LYS:HD2	1.95	0.66
2:A:603:NPS:H11	2:A:603:NPS:OXT	1.96	0.65
1:A:117:ARG:NH2	1:A:183:ASP:OD1	2.25	0.64
1:A:49:LEU:HD11	1:A:61:ASN:HB2	1.78	0.64
1:A:433:VAL:HG22	1:A:452:TYR:CD2	2.34	0.63
1:A:466:LYS:O	1:A:468:PRO:HD3	1.98	0.63
1:A:151:ALA:HB3	1:A:152:PRO:HD3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:GLU:OE2	1:A:80:LEU:CG	2.43	0.62
1:A:408:LEU:HD21	1:A:424:VAL:HA	1.82	0.62
1:A:140:TYR:O	1:A:144:ARG:HD3	2.00	0.61
1:A:304:ALA:HB1	3:A:719:HOH:O	2.00	0.61
1:A:372:LYS:C	3:A:780:HOH:O	2.42	0.61
1:A:59:ALA:HB3	1:A:62:CYS:SG	2.41	0.61
1:A:49:LEU:O	1:A:53:CYS:SG	2.60	0.60
1:A:433:VAL:HG22	1:A:452:TYR:HD2	1.66	0.60
1:A:485:ARG:HD2	1:A:485:ARG:C	2.27	0.60
1:A:224:PRO:O	1:A:336:ARG:NH1	2.36	0.59
2:A:603:NPS:OXT	2:A:603:NPS:C11	2.51	0.59
1:A:269:GLU:OE1	1:A:269:GLU:N	2.29	0.59
1:A:348:ARG:HG2	1:A:482:VAL:CG1	2.33	0.59
1:A:157:TYR:HD1	1:A:185:LEU:HD11	1.68	0.59
1:A:472:LYS:HG3	3:A:735:HOH:O	2.01	0.59
1:A:505:GLU:O	1:A:508:THR:HG22	2.02	0.59
1:A:464:HIS:C	3:A:776:HOH:O	2.46	0.58
1:A:42:LEU:O	1:A:46:VAL:HG23	2.02	0.58
1:A:408:LEU:HD22	1:A:530:VAL:CG2	2.34	0.58
1:A:41:LYS:NZ	3:A:734:HOH:O	2.35	0.58
1:A:457:LEU:HD22	1:A:488:PHE:CD2	2.39	0.57
1:A:38:GLU:HB3	1:A:77:LEU:HD11	1.86	0.57
1:A:196:GLU:OE2	1:A:242:HIS:ND1	2.33	0.57
1:A:331:LEU:O	1:A:335:SER:HB2	2.04	0.57
1:A:446:LEU:O	1:A:447:PRO:C	2.44	0.57
1:A:347:LEU:HB3	1:A:482:VAL:HG21	1.87	0.57
1:A:118:PRO:HD2	1:A:123:LEU:HD13	1.87	0.56
1:A:509:PHE:HE2	1:A:551:PHE:CZ	2.22	0.56
1:A:502:PHE:CE2	1:A:576:VAL:HG13	2.40	0.56
1:A:567:CYS:SG	1:A:568:PHE:N	2.70	0.56
1:A:484:ARG:O	1:A:487:CYS:HB3	2.06	0.56
1:A:516:LEU:HB3	1:A:520:GLU:CB	2.35	0.56
1:A:75:CYS:C	1:A:78:PRO:HD2	2.31	0.55
1:A:45:GLU:HB3	1:A:73:LYS:CE	2.37	0.55
1:A:441:PRO:HG2	1:A:444:GLU:HG3	1.87	0.55
1:A:156:TYR:CZ	1:A:288:HIS:CD2	2.95	0.55
1:A:118:PRO:HD2	1:A:123:LEU:CD1	2.37	0.55
1:A:45:GLU:HB3	1:A:73:LYS:HE3	1.89	0.54
1:A:439:LYS:HD3	1:A:440:HIS:HD2	1.72	0.54
1:A:119:GLU:O	1:A:122:VAL:N	2.39	0.54
1:A:45:GLU:OE2	1:A:73:LYS:HD2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:603:NPS:H122	3:A:804:HOH:O	2.07	0.54
1:A:441:PRO:HG2	1:A:444:GLU:CG	2.38	0.53
1:A:53:CYS:O	1:A:54:VAL:C	2.48	0.53
1:A:545:LYS:HG2	2:A:603:NPS:OXT	2.09	0.53
1:A:19:PHE:C	1:A:19:PHE:CD2	2.87	0.52
1:A:38:GLU:CD	1:A:80:LEU:HG	2.34	0.52
1:A:363:THR:HG22	1:A:365:ASP:N	2.13	0.52
1:A:153:GLU:O	1:A:156:TYR:HB3	2.09	0.52
1:A:135:PHE:HA	1:A:138:TYR:HB3	1.92	0.52
1:A:558:CYS:HB2	1:A:568:PHE:HE1	1.75	0.52
1:A:198:LEU:HA	1:A:458:ASN:ND2	2.25	0.51
1:A:332:TYR:O	1:A:336:ARG:HG3	2.11	0.51
1:A:310:VAL:CG1	1:A:371:ALA:HA	2.40	0.51
1:A:571:GLU:HG3	1:A:574:LYS:NZ	2.25	0.51
1:A:348:ARG:O	1:A:351:LYS:HB3	2.11	0.50
1:A:107:ASP:OD1	1:A:107:ASP:C	2.54	0.50
1:A:545:LYS:HG3	2:A:603:NPS:H103	1.94	0.50
1:A:131:GLU:OE1	1:A:162:LYS:HE2	2.12	0.50
1:A:525:LYS:CE	1:A:552:THR:OG1	2.56	0.50
1:A:30:TYR:HE1	1:A:103:LEU:CD2	2.25	0.50
1:A:81:ARG:HG3	1:A:83:THR:HG23	1.92	0.50
1:A:161:TYR:CE1	1:A:182:LEU:HD11	2.47	0.50
1:A:475:LYS:NZ	1:A:479:GLU:OE1	2.29	0.50
1:A:249:ASP:HB3	1:A:252:GLU:CD	2.36	0.50
1:A:347:LEU:HB3	1:A:482:VAL:CG2	2.42	0.50
1:A:363:THR:HG22	1:A:364:ASP:N	2.27	0.49
1:A:348:ARG:HG2	1:A:482:VAL:HG13	1.94	0.49
1:A:77:LEU:O	1:A:80:LEU:O	2.29	0.49
1:A:198:LEU:HD13	1:A:458:ASN:HB2	1.95	0.49
1:A:348:ARG:CG	1:A:482:VAL:HG13	2.43	0.49
1:A:457:LEU:O	1:A:460:LEU:HB3	2.12	0.49
1:A:508:THR:C	1:A:509:PHE:CG	2.91	0.49
1:A:34:CYS:SG	1:A:84:TYR:OH	2.25	0.49
1:A:97:GLU:O	1:A:101:CYS:HB2	2.13	0.48
1:A:509:PHE:CE2	1:A:551:PHE:CZ	3.00	0.48
1:A:156:TYR:CZ	1:A:160:LYS:HD2	2.48	0.48
1:A:214:TRP:HE1	1:A:343:VAL:HG21	1.76	0.48
1:A:544:LEU:HB3	2:A:603:NPS:H101	1.95	0.48
1:A:274:HIS:CD2	1:A:296:ASP:HA	2.48	0.48
1:A:311:GLU:O	1:A:312:ASP:C	2.57	0.48
1:A:33:LYS:HB2	3:A:805:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:CYS:HG	1:A:84:TYR:HH	0.55	0.47
1:A:420:THR:HG21	1:A:527:THR:HG23	1.97	0.47
1:A:558:CYS:HB2	1:A:568:PHE:CE1	2.49	0.47
1:A:213:ALA:HB2	2:A:602:NPS:C13	2.44	0.47
1:A:196:GLU:OE1	1:A:196:GLU:HA	2.14	0.47
1:A:151:ALA:HB2	1:A:250:LEU:HD13	1.96	0.47
1:A:209:ARG:NH2	1:A:324:ASP:OD1	2.48	0.47
1:A:417:GLN:HG2	1:A:470:SER:HB2	1.97	0.47
1:A:119:GLU:HA	1:A:119:GLU:OE2	2.13	0.46
1:A:440:HIS:HB3	1:A:441:PRO:HD2	1.97	0.46
1:A:150:TYR:HB2	1:A:196:GLU:HG2	1.97	0.46
1:A:13:ASP:OD2	1:A:255:ASP:OD2	2.34	0.46
1:A:372:LYS:O	1:A:373:VAL:C	2.57	0.46
1:A:74:ILE:O	1:A:77:LEU:HB3	2.15	0.46
1:A:82:ASP:HB3	1:A:85:GLY:HA3	1.97	0.46
1:A:95:GLU:HB3	1:A:96:PRO:HA	1.97	0.46
1:A:317:LYS:HG2	1:A:321:GLU:OE1	2.16	0.46
1:A:4:LYS:HD2	1:A:4:LYS:HA	1.53	0.46
1:A:503:ASN:O	1:A:504:ALA:C	2.59	0.46
1:A:387:LEU:HD12	1:A:387:LEU:HA	1.72	0.45
1:A:74:ILE:O	1:A:74:ILE:CG2	2.64	0.45
1:A:439:LYS:HD3	1:A:440:HIS:CD2	2.49	0.45
1:A:77:LEU:HD12	1:A:77:LEU:HA	1.84	0.45
1:A:257:ARG:CZ	1:A:287:ALA:HB1	2.47	0.45
1:A:372:LYS:HB2	1:A:376:GLU:OE1	2.16	0.45
1:A:340:ASP:O	1:A:447:PRO:HD3	2.16	0.44
1:A:414:LYS:HG2	1:A:491:LEU:HB2	1.99	0.44
1:A:441:PRO:CG	1:A:444:GLU:HG3	2.48	0.44
1:A:580:LYS:CB	3:A:795:HOH:O	2.37	0.44
1:A:94:LYS:O	1:A:97:GLU:HG2	2.16	0.44
1:A:449:VAL:HG11	2:A:601:NPS:H123	2.00	0.44
1:A:480:SER:HG	1:A:483:ASP:HB2	1.81	0.44
1:A:112:LEU:HA	1:A:113:PRO:HD2	1.75	0.44
1:A:157:TYR:CD1	1:A:185:LEU:HD11	2.49	0.44
1:A:484:ARG:HH11	1:A:484:ARG:HD3	1.64	0.44
1:A:219:LEU:HD22	1:A:223:PHE:HE2	1.82	0.44
1:A:151:ALA:CB	1:A:250:LEU:HD13	2.48	0.44
1:A:502:PHE:HE2	1:A:576:VAL:HG13	1.81	0.44
1:A:574:LYS:HB3	1:A:574:LYS:HE2	1.73	0.44
1:A:501:GLU:HA	1:A:501:GLU:OE2	2.18	0.43
1:A:29:GLN:HG2	1:A:147:PRO:HA	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:PHE:CZ	1:A:162:LYS:HB2	2.54	0.43
1:A:146:HIS:C	1:A:148:TYR:H	2.27	0.43
1:A:313:LYS:HG2	1:A:314:ASP:N	2.34	0.43
1:A:524:LYS:HD2	1:A:524:LYS:HA	1.56	0.43
1:A:81:ARG:HA	1:A:81:ARG:HD2	1.75	0.43
1:A:199:ARG:HD2	1:A:242:HIS:CE1	2.54	0.43
1:A:224:PRO:HD2	1:A:296:ASP:HB3	1.99	0.43
1:A:345:LEU:O	1:A:346:LEU:C	2.59	0.43
1:A:505:GLU:C	1:A:507:PHE:H	2.26	0.43
1:A:50:ALA:O	1:A:54:VAL:HG23	2.19	0.43
1:A:151:ALA:HB3	1:A:152:PRO:CD	2.46	0.43
1:A:214:TRP:NE1	3:A:784:HOH:O	2.23	0.43
1:A:508:THR:HG23	1:A:509:PHE:N	2.32	0.42
1:A:366:PRO:HG2	3:A:772:HOH:O	2.18	0.42
1:A:433:VAL:HG11	1:A:449:VAL:HG13	2.02	0.42
1:A:31:LEU:HB3	1:A:34:CYS:SG	2.59	0.42
1:A:374:LEU:O	1:A:377:PHE:HB2	2.19	0.42
1:A:153:GLU:O	1:A:154:LEU:C	2.60	0.42
1:A:392:CYS:SG	2:A:601:NPS:H121	2.59	0.42
1:A:414:LYS:HG2	1:A:491:LEU:CB	2.50	0.42
1:A:513:ILE:HD11	1:A:555:LEU:HD22	2.01	0.42
1:A:221:GLN:NE2	1:A:341:TYR:O	2.52	0.42
1:A:374:LEU:O	1:A:375:ASP:C	2.63	0.42
1:A:529:LEU:HA	1:A:532:LEU:HD12	2.01	0.42
1:A:119:GLU:O	1:A:120:ALA:C	2.62	0.42
1:A:137:HIS:O	1:A:141:GLU:HG2	2.19	0.42
1:A:449:VAL:CG1	2:A:601:NPS:H123	2.50	0.42
1:A:9:HIS:NE2	1:A:13:ASP:OD2	2.52	0.42
1:A:224:PRO:CD	1:A:296:ASP:HB3	2.50	0.41
1:A:308:GLU:HB3	1:A:309:PHE:CD2	2.55	0.41
1:A:275:LEU:O	1:A:276:LYS:C	2.60	0.41
1:A:74:ILE:O	1:A:74:ILE:HG22	2.21	0.41
1:A:116:ALA:O	1:A:118:PRO:HD3	2.21	0.41
1:A:66:LEU:HD23	1:A:66:LEU:HA	1.95	0.41
1:A:95:GLU:HB3	3:A:778:HOH:O	2.21	0.41
1:A:414:LYS:HE2	1:A:488:PHE:O	2.21	0.41
1:A:485:ARG:HB3	1:A:486:PRO:HD3	2.03	0.41
1:A:310:VAL:HG13	1:A:371:ALA:HA	2.02	0.41
1:A:434:GLY:HA2	1:A:438:CYS:SG	2.61	0.41
1:A:485:ARG:HD2	1:A:485:ARG:O	2.20	0.41
1:A:42:LEU:HD22	1:A:73:LYS:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:LEU:HD22	1:A:223:PHE:CE2	2.56	0.40
1:A:180:PRO:HG2	1:A:181:LYS:NZ	2.36	0.40
1:A:302:LEU:HA	1:A:303:PRO:HD2	1.87	0.40
1:A:571:GLU:O	1:A:575:LEU:N	2.54	0.40
1:A:251:LEU:O	1:A:252:GLU:C	2.63	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	584/584 (100%)	540 (92%)	42 (7%)	2 (0%)	36 54

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	120	ALA
1	A	147	PRO

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	512/510 (100%)	445 (87%)	67 (13%)	4 6

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	HIS
1	A	4	LYS
1	A	19	PHE
1	A	31	LEU
1	A	33	LYS
1	A	41	LYS
1	A	80	LEU
1	A	83	THR
1	A	93	LYS
1	A	94	LYS
1	A	97	GLU
1	A	117	ARG
1	A	123	LEU
1	A	125	LYS
1	A	132	LYS
1	A	152	PRO
1	A	159	GLN
1	A	181	LYS
1	A	190	LEU
1	A	191	ILE
1	A	209	ARG
1	A	227[A]	ASP
1	A	227[B]	ASP
1	A	240	LYS
1	A	243	LYS
1	A	245	CYS
1	A	252	GLU
1	A	262	LYS
1	A	269	GLU
1	A	277	GLU
1	A	297	GLU
1	A	305	VAL
1	A	307	GLU
1	A	313	LYS
1	A	329	LYS
1	A	336	ARG
1	A	372	LYS
1	A	386	ASN
1	A	393	GLU
1	A	397	GLN
1	A	413	LYS
1	A	417	GLN

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Mol	Chain	Res	Type
1	A	435	SER
1	A	439	LYS
1	A	455	VAL
1	A	462	VAL
1	A	470	SER
1	A	471	GLU
1	A	479	GLU
1	A	482	VAL
1	A	484	ARG
1	A	486	PRO
1	A	495	GLU
1	A	496	THR
1	A	506	THR
1	A	508	THR
1	A	510	HIS
1	A	513	ILE
1	A	515	THR
1	A	524	LYS
1	A	552	THR
1	A	567	CYS
1	A	571	GLU
1	A	574	LYS
1	A	575	LEU
1	A	580	LYS
1	A	582	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	ASN
1	A	146	HIS
1	A	204	GLN
1	A	378	GLN
1	A	390	GLN
1	A	391	ASN
1	A	405	ASN
1	A	440	HIS
1	A	503	ASN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

3 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	A	603	-	18,18,18	1.51	4 (22%)	25,25,25	0.97	0
2	NPS	A	602	-	18,18,18	1.97	8 (44%)	25,25,25	0.95	0
2	NPS	A	601	-	18,18,18	1.55	5 (27%)	25,25,25	0.93	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NPS	A	603	-	-	8/10/10/10	0/2/2/2
2	NPS	A	602	-	-	6/10/10/10	0/2/2/2
2	NPS	A	601	-	-	6/10/10/10	0/2/2/2

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	602	NPS	OXT-C15	3.92	1.33	1.22
2	A	602	NPS	C3-C2	3.15	1.43	1.36
2	A	602	NPS	C14-C15	3.03	1.60	1.52
2	A	603	NPS	OXT-C15	3.01	1.31	1.22
2	A	602	NPS	O2-C1	2.78	1.43	1.37
2	A	601	NPS	C13-C5	-2.62	1.36	1.42
2	A	601	NPS	C3-C2	2.40	1.41	1.36
2	A	601	NPS	O2-C1	2.36	1.42	1.37
2	A	603	NPS	C10-C14	-2.29	1.45	1.52
2	A	601	NPS	OXT-C15	2.28	1.28	1.22
2	A	602	NPS	C6-C5	2.25	1.47	1.42
2	A	602	NPS	C7-C8	2.24	1.41	1.37
2	A	603	NPS	C8-C14	-2.11	1.49	1.52
2	A	603	NPS	C3-C2	2.11	1.41	1.36
2	A	602	NPS	C13-C11	2.06	1.41	1.36
2	A	602	NPS	C11-C8	2.05	1.42	1.39
2	A	601	NPS	C10-C14	-2.03	1.46	1.52

There are no bond angle outliers.

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	602	NPS	C2-C1-O2-C12
2	A	602	NPS	C6-C1-O2-C12
2	A	603	NPS	C6-C1-O2-C12
2	A	603	NPS	C2-C1-O2-C12
2	A	601	NPS	C8-C14-C15-OXT
2	A	601	NPS	C8-C14-C15-O
2	A	601	NPS	C6-C1-O2-C12
2	A	601	NPS	C2-C1-O2-C12
2	A	603	NPS	C8-C14-C15-OXT
2	A	603	NPS	C15-C14-C8-C11
2	A	601	NPS	C10-C14-C15-O
2	A	603	NPS	C8-C14-C15-O
2	A	601	NPS	C10-C14-C15-OXT
2	A	603	NPS	C15-C14-C8-C7
2	A	603	NPS	C10-C14-C15-OXT
2	A	602	NPS	C8-C14-C15-OXT
2	A	602	NPS	C10-C14-C15-OXT
2	A	603	NPS	C10-C14-C15-O
2	A	602	NPS	C10-C14-C8-C7

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Mol	Chain	Res	Type	Atoms
2	A	602	NPS	C10-C14-C15-O

There are no ring outliers.

3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	603	NPS	6	0
2	A	602	NPS	2	0
2	A	601	NPS	3	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	583/584 (99%)	-0.35	7 (1%) 76 75	29, 52, 100, 154	3 (0%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	ALA	2.8
1	A	561	ALA	2.8
1	A	165	LEU	2.6
1	A	509	PHE	2.3
1	A	104[A]	HIS	2.1
1	A	172	ALA	2.1
1	A	504	ALA	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(Å ²)	Q<0.9
2	NPS	A	603	17/17	0.78	0.14	50,61,76,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NPS	A	602	17/17	0.82	0.16	51,60,75,80	0
2	NPS	A	601	17/17	0.95	0.08	39,44,50,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.