



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 04:41 am BST

PDB ID : 4PO0  
Title : Crystal Structure of Leporine Serum Albumin in complex with naproxen  
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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](mailto: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.

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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

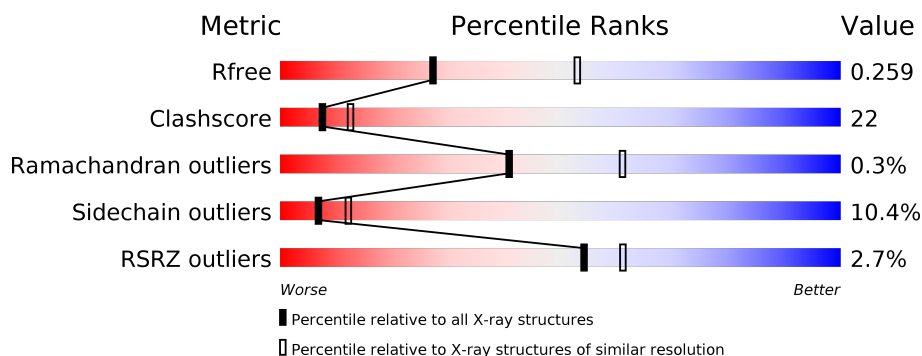
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.73 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))
$R_{free}$	130704	1271 (2.76-2.72)
Clashscore	141614	1322 (2.76-2.72)
Ramachandran outliers	138981	1297 (2.76-2.72)
Sidechain outliers	138945	1298 (2.76-2.72)
RSRZ outliers	127900	1243 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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](#)

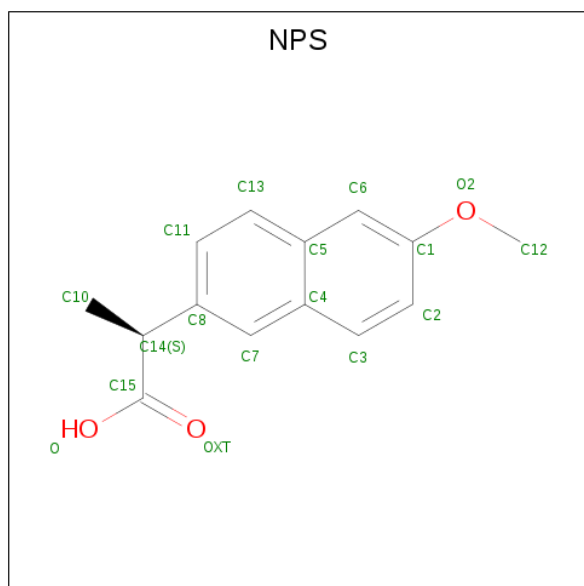
There are 3 unique types of molecules in this entry. The entry contains 4813 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (three-letter code: NPS) (formula: C<sub>14</sub>H<sub>14</sub>O<sub>3</sub>).



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	A	1	Total	C	O	0	0
			17	14	3		

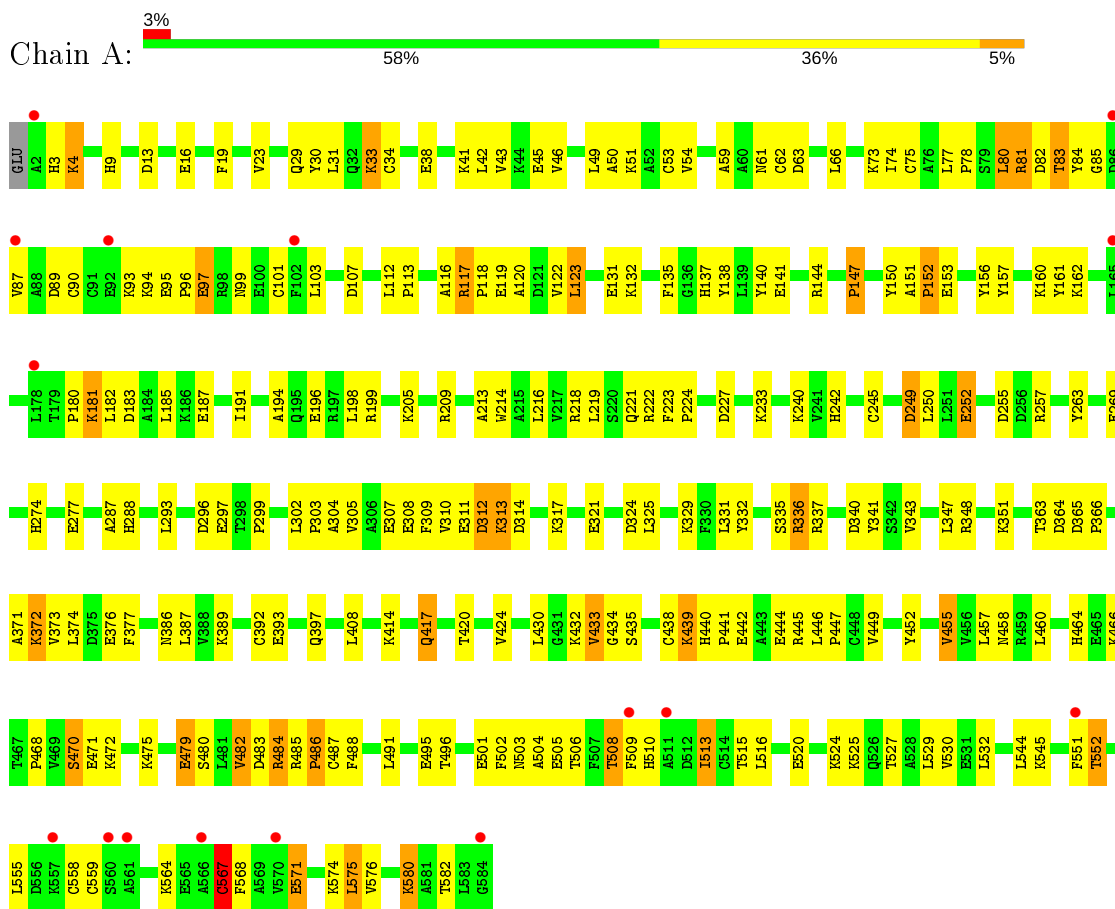
- Molecule 3 is water.

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 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 ( $\text{RSRZ} > 2$ ). 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, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	54.7	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 47.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4813	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

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	0.83	0/4752	1.01	10/6424 (0.2%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	205	LYS	CD-CE-NZ	-5.72	98.55	111.70
1	A	218	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	A	216	LEU	CA-CB-CG	5.42	127.78	115.30
1	A	337	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	A	567	CYS	CA-CB-SG	-5.22	104.61	114.00
1	A	249	ASP	CB-CG-OD1	-5.22	113.60	118.30
1	A	433	VAL	CB-CA-C	-5.22	101.49	111.40
1	A	63	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	312	ASP	CB-CG-OD1	5.09	122.88	118.30
1	A	325	LEU	CA-CB-CG	-5.07	103.64	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4641	0	4544	201	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	51	0	39	11	0
3	A	121	0	0	15	0
All	All	4813	0	4583	205	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 22.

All (205) 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:87:VAL:HG13	1:A:90:CYS:SG	2.30	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:224:PRO:HB2	1:A:299:PRO:HD3	1.76	0.68
1:A:45:GLU:HG3	3:A:734:HOH:O	1.94	0.68
1:A:233:LYS:HE2	1:A:263:TYR:CE2	2.29	0.67
1:A:95:GLU:OE1	1:A:99:ASN:HB2	1.95	0.67
1:A:78:PRO:HG3	1:A:82:ASP:OD1	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:PRO:HA	1:A:82:ASP:OD2	1.95	0.66
1:A:269:GLU:H	1:A:269:GLU:CD	1.98	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:567:CYS:SG	1:A:568:PHE:N	2.70	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
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: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:224:PRO:O	1:A:336:ARG:NH1	2.36	0.59
2:A:603:NPS:C11	2:A:603:NPS:OXT	2.51	0.59
1:A:269:GLU:N	1:A:269:GLU:OE1	2.29	0.59
1:A:348:ARG:HG2	1:A:482:VAL:CG1	2.33	0.59
1:A:372:LYS:HB3	1:A:372:LYS:HZ3	1.65	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:408:LEU:HD22	1:A:530:VAL:CG2	2.34	0.58
1:A:42:LEU:O	1:A:46:VAL:HG23	2.02	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:347:LEU:HB3	1:A:482:VAL:HG21	1.87	0.57
1:A:372:LYS:C	3:A:780:HOH:O	2.42	0.56
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: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:45:GLU:HB3	1:A:73:LYS:CE	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:485:ARG:HD2	1:A:485:ARG:C	2.27	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
1:A:464:HIS:C	3:A:776:HOH:O	2.46	0.54
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:545:LYS:HG2	2:A:603:NPS:OXT	2.09	0.53
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:446:LEU:O	1:A:447:PRO:C	2.44	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:372:LYS:HZ2	1:A:372:LYS:HB3	1.69	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:75:CYS:C	1:A:78:PRO:HD2	2.31	0.51
1:A:348:ARG:O	1:A:351:LYS:HB3	2.11	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: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:457:LEU:O	1:A:460:LEU:HB3	2.12	0.49
1:A:348:ARG:CG	1:A:482:VAL:HG13	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:CYS:O	1:A:54:VAL:C	2.48	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:19:PHE:C	1:A:19:PHE:CD2	2.87	0.48
1:A:33:LYS:HB2	3:A:805:HOH:O	2.14	0.47
1:A:196:GLU:HA	1:A:196:GLU:OE1	2.14	0.47
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: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:107:ASP:OD1	1:A:107:ASP:C	2.54	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: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:387:LEU:HA	1:A:387:LEU:HD12	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:249:ASP:HB3	1:A:252:GLU:CD	2.36	0.45
1:A:77:LEU:HA	1:A:77:LEU:HD12	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:38:GLU:CD	1:A:80:LEU:HG	2.34	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:480:SER:HG	1:A:483:ASP:HB2	1.81	0.44
1:A:449:VAL:HG11	2:A:601:NPS:H123	2.00	0.44
1:A:94:LYS:O	1:A:97:GLU:HG2	2.16	0.44
1:A:112:LEU:HA	1:A:113:PRO:HD2	1.75	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:508:THR:C	1:A:509:PHE:CG	2.91	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:574:LYS:HE2	1:A:574:LYS:HB3	1.73	0.44
1:A:502:PHE:HE2	1:A:576:VAL:HG13	1.81	0.44
1:A:501:GLU:HA	1:A:501:GLU:OE2	2.18	0.43
1:A:135:PHE:CZ	1:A:162:LYS:HB2	2.54	0.43
1:A:29:GLN:HG2	1:A:147:PRO:HA	1.99	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: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:311:GLU:O	1:A:312:ASP:C	2.57	0.43
1:A:81:ARG:HD2	1:A:81:ARG:HA	1.75	0.43
1:A:151:ALA:HB3	1:A:152:PRO:CD	2.46	0.43
1:A:50:ALA:O	1:A:54:VAL:HG23	2.19	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: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:392:CYS:SG	2:A:601:NPS:H121	2.59	0.42
1:A:221:GLN:NE2	1:A:341:TYR:O	2.52	0.42
1:A:529:LEU:HA	1:A:532:LEU:HD12	2.01	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:372:LYS:O	1:A:373:VAL:C	2.57	0.41
1:A:116:ALA:O	1:A:118:PRO:HD3	2.21	0.41
1:A:503:ASN:O	1:A:504:ALA:C	2.59	0.41
1:A:74:ILE:HG22	1:A:74:ILE:O	2.21	0.41
1:A:485:ARG:HB3	1:A:486:PRO:HD3	2.03	0.41
1:A:414:LYS:HE2	1:A:488:PHE:O	2.21	0.41
1:A:66:LEU:HA	1:A:66:LEU:HD23	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:GLU:HB3	3:A:778:HOH:O	2.21	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:O	1:A:485:ARG:HD2	2.20	0.41
1:A:219:LEU:HD22	1:A:223:PHE:CE2	2.56	0.40
1:A:42:LEU:HD22	1:A:73:LYS:HB3	2.03	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

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%)	41 61

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%)	458 (90%)	54 (10%)	7 12

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	HIS
1	A	4	LYS
1	A	33	LYS
1	A	80	LEU
1	A	81	ARG
1	A	83	THR
1	A	89	ASP
1	A	93	LYS
1	A	97	GLU
1	A	117	ARG
1	A	123	LEU
1	A	132	LYS
1	A	152	PRO
1	A	181	LYS
1	A	227[A]	ASP
1	A	227[B]	ASP
1	A	240	LYS
1	A	245	CYS
1	A	252	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	389	LYS
1	A	393	GLU
1	A	397	GLN
1	A	417	GLN
1	A	435	SER
1	A	439	LYS
1	A	455	VAL
1	A	470	SER
1	A	471	GLU
1	A	479	GLU

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Mol	Chain	Res	Type
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	552	THR
1	A	567	CYS
1	A	571	GLU
1	A	575	LEU
1	A	580	LYS
1	A	582	THR

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

Mol	Chain	Res	Type
1	A	204	GLN
1	A	378	GLN
1	A	440	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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

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	601	-	15,18,18	1.78	4 (26%)	21,25,25	0.85	0
2	NPS	A	602	-	15,18,18	1.75	6 (40%)	21,25,25	0.85	0
2	NPS	A	603	-	15,18,18	1.73	3 (20%)	21,25,25	0.90	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	601	-	-	2/6/10/10	0/2/2/2
2	NPS	A	602	-	-	2/6/10/10	0/2/2/2
2	NPS	A	603	-	-	4/6/10/10	0/2/2/2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	603	NPS	C10-C14	-4.45	1.45	1.53
2	A	601	NPS	C10-C14	-4.00	1.46	1.53
2	A	602	NPS	C3-C2	3.27	1.43	1.36
2	A	602	NPS	O2-C1	2.64	1.43	1.37
2	A	601	NPS	C3-C2	2.49	1.41	1.36
2	A	601	NPS	C13-C5	-2.35	1.36	1.41
2	A	601	NPS	O2-C1	2.23	1.42	1.37
2	A	603	NPS	C3-C2	2.20	1.41	1.36
2	A	602	NPS	C6-C5	2.19	1.47	1.42
2	A	602	NPS	C7-C8	2.19	1.41	1.37
2	A	603	NPS	C8-C14	-2.15	1.49	1.52
2	A	602	NPS	C13-C11	2.14	1.41	1.36
2	A	602	NPS	C11-C8	2.06	1.42	1.39

There are no bond angle outliers.

There are no chirality outliers.



All (8) 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	C6-C1-O2-C12
2	A	601	NPS	C2-C1-O2-C12
2	A	603	NPS	C15-C14-C8-C11
2	A	603	NPS	C15-C14-C8-C7

There are no ring outliers.

3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	NPS	3	0
2	A	602	NPS	2	0
2	A	603	NPS	6	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	583/584 (99%)	-0.15	16 (2%) 54 61	30, 52, 100, 154	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	ALA	6.1
1	A	509	PHE	4.7
1	A	561	ALA	4.1
1	A	511	ALA	3.5
1	A	560	SER	3.5
1	A	87	VAL	3.5
1	A	165	LEU	3.2
1	A	86	ASP	3.1
1	A	551	PHE	2.9
1	A	178	LEU	2.8
1	A	92	GLU	2.8
1	A	584	GLY	2.6
1	A	570	VAL	2.5
1	A	557	LYS	2.5
1	A	566	ALA	2.3
1	A	102	PHE	2.2

### 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, 95<sup>th</sup> 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	NPS	A	602	17/17	0.80	0.26	51,60,75,80	0
2	NPS	A	603	17/17	0.88	0.28	50,61,76,78	0
2	NPS	A	601	17/17	0.95	0.22	39,44,50,57	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.