Full wwPDB X-ray Structure Validation Report ⓘ

Dec 8, 2023 – 07:18 am GMT

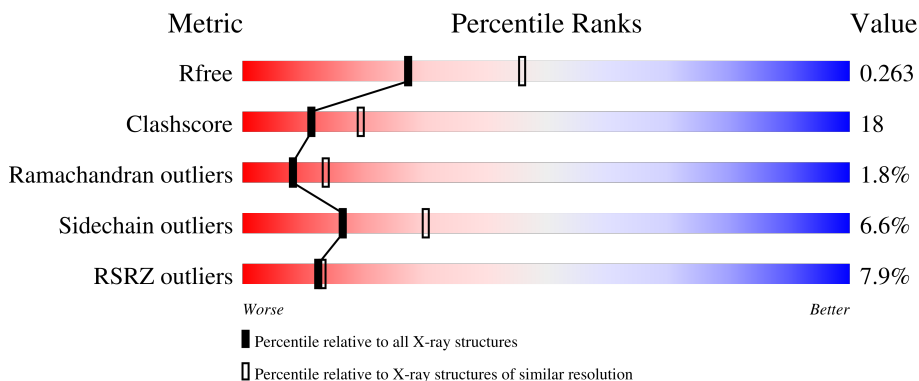|		
PDB ID	:	2VDB
Title	:	Structure of human serum albumin with S-naproxen and the GA module
Authors	:	Lejon, S.; Cramer, J.F.; Nordberg, P.A.
Deposited on	:	2007-10-04
Resolution	:	2.52 Å(reported)

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1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
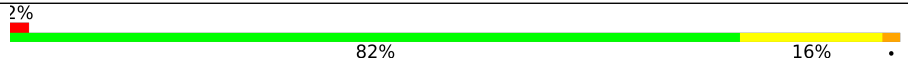*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.52 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	Percentile Ranks	Value
Rfree		0.263
Clashscore		18
Ramachandran outliers		1.8%
Sidechain outliers		6.6%
RSRZ outliers		7.9%

Worse ——— *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5743 (2.54-2.50)
Clashscore	141614	6463 (2.54-2.50)
Ramachandran outliers	138981	6335 (2.54-2.50)
Sidechain outliers	138945	6337 (2.54-2.50)
RSRZ outliers	127900	5630 (2.54-2.50)

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 <=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	579	8% / 65% / 28% / 5% ··
2	B	55	2% / 82% / 16% ·

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 4872 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	574	4346	2751	741	814	40	0	0	0

- Molecule 2 is a protein called PEPTOSTREPTOCOCCAL ALBUMIN-BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	55	437	279	74	83	1	0	0	0

- Molecule 3 is DECANOIC ACID (three-letter code: DKA) (formula: $C_{10}H_{20}O_2$).
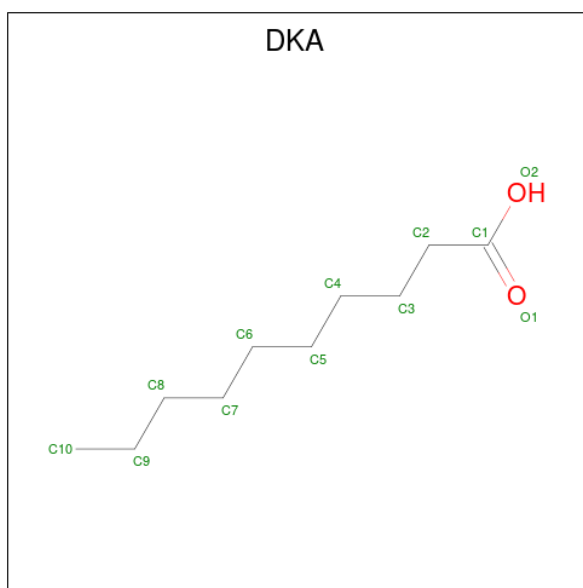
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	12	10	2	0	0
3	A	1	12	10	2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 12	C 10	O 2	0	0
3	A	1	Total 12	C 10	O 2	0	0
3	A	1	Total 12	C 10	O 2	0	0
3	A	1	Total 12	C 10	O 2	0	0

- Molecule 4 is (2S)-2-(6-methoxynaphthalen-2-yl)propanoic acid (three-letter code: NPS) (formula: $C_{14}H_{14}O_3$).
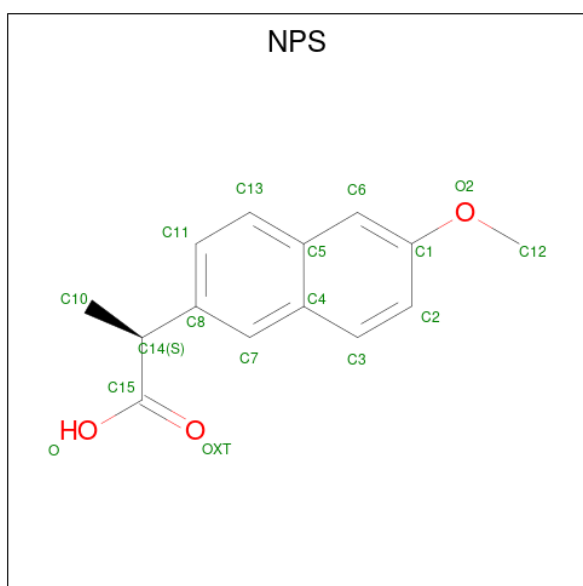
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 17	C 14	O 3	0	0

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
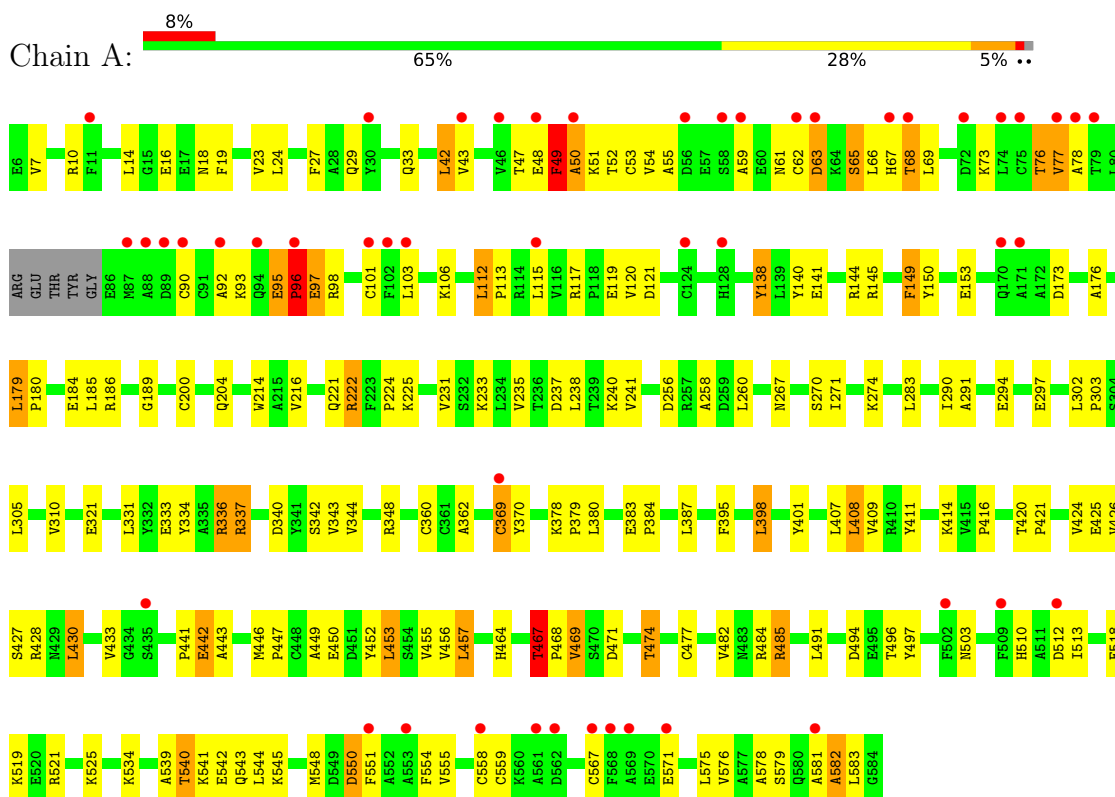
• Molecule 2: PEPTOSTREPTOCOCCAL ALBUMIN-BINDING PROTEIN
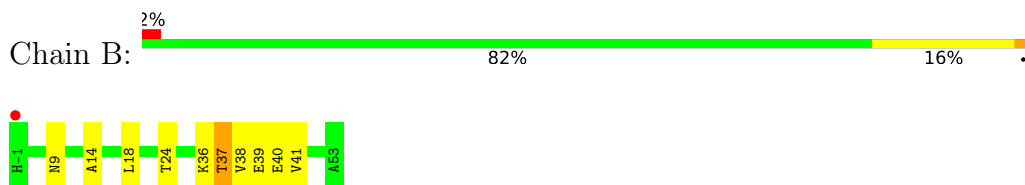
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	190.51Å 49.46Å 79.93Å 90.00° 93.00° 90.00°	Depositor
Resolution (Å)	94.92 – 2.52 47.87 – 2.52	Depositor EDS
% Data completeness (in resolution range)	96.7 (94.92-2.52) 96.7 (47.87-2.52)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.09 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.234 , 0.280 0.224 , 0.263	Depositor DCC
R_{free} test set	1273 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å^2)	50.9	Xtriage
Anisotropy	0.189	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 69.0	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	4872	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.64% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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, DKA

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	0.78	9/4433 (0.2%)	0.70	7/6019 (0.1%)
2	B	0.53	0/443	0.61	0/594
All	All	0.76	9/4876 (0.2%)	0.69	7/6613 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	63	ASP	CG-OD1	21.56	1.75	1.25
1	A	63	ASP	CG-OD2	14.16	1.57	1.25
1	A	78	ALA	C-O	10.32	1.43	1.23
1	A	76	THR	C-O	8.77	1.40	1.23
1	A	65	SER	CB-OG	8.24	1.52	1.42
1	A	78	ALA	C-N	7.64	1.51	1.34
1	A	76	THR	CB-CG2	6.69	1.74	1.52
1	A	73	LYS	C-O	5.76	1.34	1.23
1	A	369	CYS	CB-SG	5.46	1.91	1.82

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	63	ASP	CB-CG-OD2	-11.70	107.77	118.30
1	A	337	ARG	NE-CZ-NH2	-6.72	116.94	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	336	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	A	63	ASP	OD1-CG-OD2	5.56	133.87	123.30
1	A	49	PHE	N-CA-C	-5.55	96.03	111.00
1	A	582	ALA	CB-CA-C	-5.53	101.80	110.10
1	A	337	ARG	NE-CZ-NH1	5.01	122.81	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	96	PRO	Peptide

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	4346	0	4076	163	0
2	B	437	0	448	9	0
3	A	72	0	114	18	0
4	A	17	0	13	3	0
All	All	4872	0	4651	168	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 18.

All (168) 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:63:ASP:OD1	1:A:63:ASP:CG	1.74	1.24
1:A:95:GLU:HG3	1:A:96:PRO:HD2	1.09	1.06
2:B:37:THR:HG22	2:B:40:GLU:H	1.16	1.06
1:A:95:GLU:CG	1:A:96:PRO:HD2	1.94	0.97
1:A:117:ARG:HE	3:A:1585:DKA:H31	1.31	0.92
1:A:19:PHE:O	1:A:23:VAL:HG23	1.74	0.88
1:A:545:LYS:HA	1:A:548:MET:HE3	1.61	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:LYS:NZ	1:A:297:GLU:O	2.13	0.82
1:A:383:GLU:OE2	1:A:485:ARG:NH1	2.15	0.79
1:A:112:LEU:HB2	1:A:113:PRO:HD2	1.69	0.73
1:A:113:PRO:O	1:A:145:ARG:NH2	2.21	0.73
1:A:68:THR:HG23	1:A:95:GLU:HG2	1.70	0.73
1:A:395:PHE:O	1:A:398:LEU:O	2.05	0.73
2:B:37:THR:HG22	2:B:40:GLU:N	2.00	0.72
1:A:558:CYS:O	1:A:559:CYS:HB2	1.89	0.72
1:A:494:ASP:OD1	1:A:496:THR:HG22	1.88	0.72
1:A:510:HIS:HB2	1:A:512:ASP:OD1	1.91	0.70
1:A:433:VAL:HG22	1:A:452:TYR:HB3	1.71	0.70
1:A:541:LYS:HA	1:A:544:LEU:HB2	1.74	0.70
1:A:283:LEU:HD23	3:A:1586:DKA:H32	1.74	0.70
1:A:401:TYR:OH	1:A:525:LYS:HE3	1.92	0.69
1:A:540:THR:O	1:A:541:LYS:HB2	1.93	0.69
1:A:449:ALA:O	1:A:453:LEU:HB2	1.91	0.69
1:A:270:SER:OG	2:B:36:LYS:HD3	1.93	0.68
1:A:581:ALA:O	1:A:582:ALA:HB3	1.94	0.67
1:A:387:LEU:HD23	3:A:1587:DKA:H62	1.77	0.66
1:A:582:ALA:O	1:A:583:LEU:HD23	1.95	0.65
1:A:27:PHE:CE2	1:A:42:LEU:HD22	2.32	0.65
1:A:333:GLU:OE1	1:A:337:ARG:NH2	2.30	0.65
1:A:291:ALA:HA	3:A:1590:DKA:H52	1.79	0.64
1:A:189:GLY:HA3	4:A:1591:NPS:H122	1.78	0.64
1:A:47:THR:HG22	1:A:48:GLU:H	1.61	0.63
1:A:430:LEU:HD13	1:A:456:VAL:HG11	1.80	0.63
1:A:117:ARG:NE	3:A:1585:DKA:H31	2.11	0.62
1:A:179:LEU:HB2	1:A:180:PRO:HD3	1.81	0.62
1:A:581:ALA:O	1:A:582:ALA:CB	2.47	0.62
1:A:189:GLY:CA	4:A:1591:NPS:H122	2.29	0.62
1:A:411:TYR:CE1	3:A:1588:DKA:H61	2.35	0.62
1:A:383:GLU:CD	1:A:485:ARG:HH12	2.03	0.61
1:A:61:ASN:O	1:A:69:LEU:HD21	2.01	0.61
2:B:37:THR:HG23	2:B:39:GLU:OE1	2.01	0.60
1:A:342:SER:HB3	1:A:446:MET:HG2	1.84	0.60
1:A:344:VAL:O	1:A:348:ARG:HG3	2.02	0.60
1:A:47:THR:C	1:A:49:PHE:H	2.06	0.59
1:A:47:THR:HG22	1:A:48:GLU:N	2.17	0.59
1:A:464:HIS:HD1	1:A:474:THR:HG23	1.66	0.59
1:A:27:PHE:CZ	1:A:42:LEU:HD22	2.39	0.58
1:A:59:ALA:HB3	1:A:62:CYS:SG	2.44	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:LEU:HB2	1:A:113:PRO:CD	2.33	0.58
1:A:93:LYS:O	1:A:98:ARG:HD3	2.05	0.57
1:A:33:GLN:HE22	1:A:112:LEU:HD23	1.70	0.57
1:A:485:ARG:HD3	3:A:1587:DKA:O1	2.04	0.57
1:A:540:THR:O	1:A:541:LYS:CB	2.52	0.56
2:B:14:ALA:O	2:B:18:LEU:HG	2.05	0.56
1:A:179:LEU:CB	1:A:180:PRO:HD3	2.35	0.56
1:A:408:LEU:HD13	1:A:427:SER:CB	2.36	0.56
1:A:200:CYS:O	1:A:204:GLN:HG3	2.06	0.56
1:A:50:ALA:C	1:A:52:THR:H	2.08	0.55
1:A:555:VAL:O	1:A:555:VAL:HG12	2.05	0.55
1:A:274:LYS:HE3	1:A:294:GLU:OE2	2.06	0.55
1:A:10:ARG:O	1:A:14:LEU:HB2	2.07	0.55
1:A:348:ARG:NH1	3:A:1587:DKA:O2	2.33	0.54
1:A:49:PHE:CZ	1:A:53:CYS:SG	3.01	0.54
1:A:283:LEU:CD2	3:A:1586:DKA:H32	2.38	0.54
1:A:467:THR:H	1:A:468:PRO:HD3	1.71	0.54
1:A:408:LEU:HD11	1:A:424:VAL:HA	1.90	0.53
1:A:95:GLU:O	1:A:96:PRO:C	2.45	0.53
1:A:241:VAL:HG22	1:A:256:ASP:HB3	1.90	0.53
1:A:409:VAL:HG12	1:A:541:LYS:HE2	1.91	0.53
1:A:407:LEU:HD13	1:A:430:LEU:HB3	1.91	0.53
1:A:117:ARG:HB2	3:A:1585:DKA:H22	1.90	0.52
1:A:513:ILE:HG12	1:A:521:ARG:HG3	1.91	0.52
1:A:303:PRO:O	1:A:337:ARG:NH1	2.42	0.52
1:A:95:GLU:OE1	1:A:98:ARG:NH2	2.43	0.52
1:A:141:GLU:O	1:A:144:ARG:HG2	2.10	0.52
1:A:47:THR:O	1:A:49:PHE:N	2.43	0.52
1:A:305:LEU:HD11	1:A:337:ARG:CZ	2.39	0.52
1:A:305:LEU:HD11	1:A:337:ARG:NE	2.25	0.51
1:A:340:ASP:O	1:A:447:PRO:HD3	2.10	0.51
1:A:231:VAL:O	1:A:235:VAL:HG23	2.11	0.51
1:A:414:LYS:NZ	1:A:491:LEU:O	2.40	0.51
1:A:477:CYS:O	1:A:484:ARG:NH2	2.44	0.51
1:A:348:ARG:HH22	3:A:1587:DKA:C1	2.23	0.50
1:A:237:ASP:HB3	1:A:260:LEU:HD13	1.94	0.50
1:A:302:LEU:HB3	1:A:337:ARG:NH1	2.27	0.49
1:A:76:THR:O	1:A:77:VAL:HB	2.12	0.49
1:A:408:LEU:HD13	1:A:427:SER:HB2	1.94	0.49
1:A:344:VAL:HG13	1:A:450:GLU:OE2	2.12	0.49
1:A:33:GLN:NE2	1:A:112:LEU:HD23	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:GLU:HB3	1:A:384:PRO:CD	2.43	0.48
1:A:411:TYR:OH	3:A:1588:DKA:O1	2.25	0.48
1:A:321:GLU:OE1	2:B:24:THR:OG1	2.28	0.48
1:A:539:ALA:HA	1:A:543:GLN:OE1	2.13	0.48
1:A:360:CYS:C	1:A:362:ALA:H	2.17	0.48
1:A:98:ARG:O	1:A:101:CYS:HB2	2.15	0.47
1:A:186:ARG:HD3	3:A:1585:DKA:O1	2.14	0.47
1:A:387:LEU:HD23	3:A:1587:DKA:C6	2.44	0.47
1:A:14:LEU:O	1:A:18:ASN:HB2	2.15	0.47
1:A:310:VAL:O	1:A:370:TYR:HE1	1.98	0.46
1:A:96:PRO:O	1:A:97:GLU:CB	2.64	0.46
1:A:47:THR:C	1:A:49:PHE:N	2.67	0.46
1:A:29:GLN:O	1:A:106:LYS:HE2	2.15	0.46
1:A:120:VAL:O	1:A:121:ASP:C	2.53	0.46
1:A:578:ALA:O	1:A:581:ALA:O	2.34	0.46
1:A:416:PRO:HG2	1:A:497:TYR:CG	2.51	0.46
1:A:464:HIS:ND1	1:A:474:THR:HG23	2.31	0.46
1:A:543:GLN:HB3	1:A:583:LEU:HD21	1.97	0.46
1:A:383:GLU:HB3	1:A:384:PRO:HD3	1.98	0.46
1:A:426:VAL:HG12	1:A:430:LEU:HD22	1.97	0.46
1:A:567:CYS:O	1:A:571:GLU:HB2	2.16	0.46
1:A:442:GLU:HG2	1:A:442:GLU:O	2.16	0.45
1:A:52:THR:C	1:A:54:VAL:N	2.69	0.45
1:A:340:ASP:N	1:A:340:ASP:OD1	2.50	0.45
1:A:407:LEU:CD1	1:A:430:LEU:HB3	2.46	0.45
1:A:66:LEU:HA	1:A:69:LEU:HD12	1.99	0.45
1:A:214:TRP:CD1	1:A:343:VAL:HG11	2.50	0.45
1:A:216:VAL:HG22	1:A:235:VAL:HG21	1.97	0.45
1:A:112:LEU:CB	1:A:113:PRO:CD	2.92	0.44
1:A:446:MET:N	1:A:447:PRO:CD	2.81	0.44
1:A:321:GLU:CD	2:B:24:THR:H	2.21	0.44
1:A:421:PRO:O	1:A:425:GLU:HG3	2.17	0.44
1:A:360:CYS:C	1:A:362:ALA:N	2.71	0.44
1:A:189:GLY:HA2	4:A:1591:NPS:H122	2.00	0.44
1:A:467:THR:N	1:A:468:PRO:HD3	2.32	0.44
1:A:416:PRO:O	1:A:534:LYS:HE2	2.18	0.44
1:A:224:PRO:O	1:A:336:ARG:HD2	2.19	0.43
1:A:340:ASP:HA	1:A:443:ALA:O	2.18	0.43
1:A:453:LEU:O	1:A:457:LEU:HB2	2.18	0.43
1:A:149:PHE:HE2	1:A:153:GLU:HB3	1.83	0.43
1:A:441:PRO:C	1:A:443:ALA:H	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:ARG:NH2	1:A:519:LYS:HG3	2.33	0.43
1:A:65:SER:HB2	1:A:67:HIS:CD2	2.53	0.43
1:A:222:ARG:HE	1:A:222:ARG:HB2	1.41	0.43
1:A:290:ILE:HG22	3:A:1590:DKA:H31	2.01	0.43
1:A:409:VAL:CG1	1:A:541:LYS:HE2	2.48	0.43
1:A:518:GLU:OE1	1:A:521:ARG:NH2	2.52	0.43
1:A:179:LEU:CB	1:A:180:PRO:CD	2.96	0.42
1:A:258:ALA:HB2	3:A:1586:DKA:H21	2.01	0.42
1:A:420:THR:HB	1:A:421:PRO:HD3	2.01	0.42
1:A:149:PHE:CD2	1:A:149:PHE:C	2.93	0.42
1:A:238:LEU:HD13	3:A:1590:DKA:H21	2.01	0.42
1:A:50:ALA:C	1:A:52:THR:N	2.73	0.42
1:A:428:ARG:HH21	1:A:519:LYS:NZ	2.17	0.42
1:A:550:ASP:HB3	1:A:575:LEU:CD1	2.50	0.42
1:A:221:GLN:O	1:A:224:PRO:HD3	2.20	0.42
1:A:380:LEU:O	1:A:384:PRO:HD2	2.19	0.42
1:A:24:LEU:HB2	1:A:43:VAL:HG21	2.02	0.42
1:A:411:TYR:CE2	1:A:430:LEU:HD23	2.55	0.42
1:A:149:PHE:O	1:A:150:TYR:C	2.58	0.41
1:A:240:LYS:HE3	1:A:240:LYS:HB2	1.59	0.41
1:A:267:ASN:O	1:A:271:ILE:HG13	2.20	0.41
1:A:233:LYS:HE3	2:B:39:GLU:HB3	2.01	0.41
1:A:428:ARG:NH2	1:A:519:LYS:NZ	2.68	0.41
1:A:52:THR:O	1:A:55:ALA:N	2.53	0.41
1:A:119:GLU:OE2	1:A:119:GLU:HA	2.21	0.41
1:A:378:LYS:HB2	1:A:379:PRO:HD3	2.01	0.41
1:A:540:THR:C	1:A:542:GLU:H	2.24	0.41
1:A:90:CYS:C	1:A:92:ALA:H	2.25	0.41
1:A:274:LYS:NZ	1:A:297:GLU:OE2	2.51	0.41
1:A:576:VAL:O	1:A:579:SER:N	2.53	0.41
1:A:420:THR:O	1:A:421:PRO:C	2.58	0.41
2:B:38:VAL:O	2:B:41:VAL:HB	2.21	0.41
1:A:348:ARG:HG2	1:A:482:VAL:CG1	2.51	0.40
1:A:138:TYR:HB3	3:A:1585:DKA:H82	2.04	0.40
1:A:428:ARG:HH21	1:A:519:LYS:HZ2	1.69	0.40
1:A:545:LYS:HA	1:A:548:MET:CE	2.41	0.40
1:A:551:PHE:O	1:A:554:PHE:HB3	2.20	0.40
1:A:173:ASP:HB3	1:A:176:ALA:HB3	2.04	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	570/579 (98%)	507 (89%)	52 (9%)	11 (2%)	8	12
2	B	53/55 (96%)	53 (100%)	0	0	100	100
All	All	623/634 (98%)	560 (90%)	52 (8%)	11 (2%)	8	14

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	GLU
1	A	77	VAL
1	A	96	PRO
1	A	467	THR
1	A	503	ASN
1	A	97	GLU
1	A	442	GLU
1	A	51	LYS
1	A	50	ALA
1	A	469	VAL
1	A	95	GLU

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	441/506 (87%)	411 (93%)	30 (7%)	16	29
2	B	45/45 (100%)	43 (96%)	2 (4%)	28	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	486/551 (88%)	454 (93%)	32 (7%)	16 30

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

Mol	Chain	Res	Type
1	A	7	VAL
1	A	42	LEU
1	A	49	PHE
1	A	68	THR
1	A	103	LEU
1	A	112	LEU
1	A	115	LEU
1	A	138	TYR
1	A	140	TYR
1	A	149	PHE
1	A	179	LEU
1	A	184	GLU
1	A	185	LEU
1	A	222	ARG
1	A	331	LEU
1	A	334	TYR
1	A	369	CYS
1	A	398	LEU
1	A	408	LEU
1	A	430	LEU
1	A	453	LEU
1	A	455	VAL
1	A	457	LEU
1	A	467	THR
1	A	469	VAL
1	A	471	ASP
1	A	474	THR
1	A	485	ARG
1	A	540	THR
1	A	550	ASP
2	B	9	ASN
2	B	37	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	33	GLN
1	A	67	HIS
1	A	111	ASN
1	A	242	HIS
1	A	318	ASN
1	A	367	HIS
1	A	440	HIS
1	A	580	GLN
2	B	42	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

7 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	#$|Z| > 2$
4	NPS	A	1591	-	18,18,18	1.49	4 (22%)	25,25,25	1.46	3 (12%)
3	DKA	A	1587	-	11,11,11	0.76	0	11,11,11	0.69	0
3	DKA	A	1590	-	11,11,11	0.69	0	11,11,11	0.81	0
3	DKA	A	1585	-	11,11,11	0.53	0	11,11,11	1.37	3 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
3	DKA	A	1589	-	11,11,11	0.74	0	11,11,11	0.63	0
3	DKA	A	1586	-	11,11,11	0.63	0	11,11,11	1.06	1 (9%)
3	DKA	A	1588	-	11,11,11	0.61	0	11,11,11	1.01	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NPS	A	1591	-	-	0/10/10/10	0/2/2/2
3	DKA	A	1587	-	-	5/9/9/9	-
3	DKA	A	1590	-	-	5/9/9/9	-
3	DKA	A	1585	-	-	4/9/9/9	-
3	DKA	A	1589	-	-	6/9/9/9	-
3	DKA	A	1586	-	-	7/9/9/9	-
3	DKA	A	1588	-	-	9/9/9/9	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1591	NPS	C6-C5	-2.72	1.35	1.42
4	A	1591	NPS	C8-C14	-2.48	1.48	1.52
4	A	1591	NPS	C13-C5	-2.42	1.36	1.41
4	A	1591	NPS	O-C15	-2.36	1.22	1.30

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1591	NPS	C8-C14-C15	4.03	120.33	108.60
4	A	1591	NPS	O2-C1-C6	-3.08	116.02	124.43
3	A	1585	DKA	C3-C2-C1	-2.81	107.39	114.47
3	A	1586	DKA	C3-C2-C1	-2.63	107.85	114.47
3	A	1585	DKA	O1-C1-C2	-2.40	115.36	123.08
4	A	1591	NPS	C11-C8-C14	-2.26	115.39	120.80
3	A	1585	DKA	O2-C1-C2	2.21	121.14	114.03

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1586	DKA	C1-C2-C3-C4
3	A	1587	DKA	C5-C6-C7-C8
3	A	1588	DKA	C6-C7-C8-C9
3	A	1586	DKA	C2-C3-C4-C5
3	A	1588	DKA	C5-C6-C7-C8
3	A	1588	DKA	C1-C2-C3-C4
3	A	1590	DKA	C3-C4-C5-C6
3	A	1585	DKA	C5-C6-C7-C8
3	A	1588	DKA	C2-C3-C4-C5
3	A	1589	DKA	C2-C3-C4-C5
3	A	1588	DKA	C4-C5-C6-C7
3	A	1585	DKA	C2-C3-C4-C5
3	A	1589	DKA	C4-C5-C6-C7
3	A	1585	DKA	C3-C4-C5-C6
3	A	1587	DKA	C1-C2-C3-C4
3	A	1587	DKA	C3-C4-C5-C6
3	A	1589	DKA	C7-C8-C9-C10
3	A	1590	DKA	C7-C8-C9-C10
3	A	1586	DKA	C4-C5-C6-C7
3	A	1588	DKA	C3-C4-C5-C6
3	A	1586	DKA	C3-C4-C5-C6
3	A	1587	DKA	C4-C5-C6-C7
3	A	1589	DKA	C5-C6-C7-C8
3	A	1589	DKA	C6-C7-C8-C9
3	A	1590	DKA	O2-C1-C2-C3
3	A	1588	DKA	O1-C1-C2-C3
3	A	1587	DKA	C6-C7-C8-C9
3	A	1585	DKA	C4-C5-C6-C7
3	A	1586	DKA	C5-C6-C7-C8
3	A	1588	DKA	O2-C1-C2-C3
3	A	1590	DKA	O1-C1-C2-C3
3	A	1586	DKA	O1-C1-C2-C3
3	A	1586	DKA	O2-C1-C2-C3
3	A	1588	DKA	C7-C8-C9-C10
3	A	1590	DKA	C6-C7-C8-C9
3	A	1589	DKA	C3-C4-C5-C6

There are no ring outliers.

6 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1591	NPS	3	0
3	A	1587	DKA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1590	DKA	3	0
3	A	1585	DKA	5	0
3	A	1586	DKA	3	0
3	A	1588	DKA	2	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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(Å²)	Q<0.9
1	A	574/579 (99%)	0.68	49 (8%)	10	11	20, 44, 57, 65	0
2	B	55/55 (100%)	0.36	1 (1%)	68	71	37, 43, 51, 70	0
All	All	629/634 (99%)	0.65	50 (7%)	12	13	20, 44, 57, 70	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	58	SER	5.5
1	A	72	ASP	5.1
1	A	77	VAL	4.8
1	A	30	TYR	4.7
1	A	101	CYS	4.5
1	A	62	CYS	4.4
1	A	78	ALA	4.1
1	A	90	CYS	4.1
1	A	102	PHE	3.9
1	A	103	LEU	3.8
1	A	561	ALA	3.7
1	A	50	ALA	3.6
1	A	63	ASP	3.4
1	A	79	THR	3.2
1	A	96	PRO	3.2
1	A	509	PHE	2.9
1	A	59	ALA	2.8
1	A	435	SER	2.8
1	A	124	CYS	2.8
1	A	581	ALA	2.8
1	A	48	GLU	2.7
1	A	92	ALA	2.7
1	A	94	GLN	2.7
1	A	88	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	171	ALA	2.7
1	A	562	ASP	2.7
1	A	558	CYS	2.6
1	A	11	PHE	2.6
1	A	553	ALA	2.5
2	B	-1	HIS	2.4
1	A	512	ASP	2.4
1	A	75	CYS	2.4
1	A	87	MET	2.3
1	A	43	VAL	2.3
1	A	89	ASP	2.3
1	A	67	HIS	2.3
1	A	369	CYS	2.2
1	A	68	THR	2.2
1	A	46	VAL	2.2
1	A	128	HIS	2.2
1	A	569	ALA	2.2
1	A	56	ASP	2.1
1	A	502	PHE	2.1
1	A	568	PHE	2.1
1	A	115	LEU	2.1
1	A	567	CYS	2.1
1	A	571	GLU	2.1
1	A	551	PHE	2.0
1	A	74	LEU	2.0
1	A	170	GLN	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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
3	DKA	A	1586	12/12	0.82	0.52	64,67,69,69	0
3	DKA	A	1590	12/12	0.83	0.19	56,56,57,57	0
3	DKA	A	1585	12/12	0.85	0.22	57,58,61,62	0
3	DKA	A	1589	12/12	0.87	0.21	51,53,56,56	0
3	DKA	A	1587	12/12	0.90	0.20	37,41,45,45	0
3	DKA	A	1588	12/12	0.91	0.24	37,38,40,40	0
4	NPS	A	1591	17/17	0.92	0.18	54,55,57,58	0

6.5 Other polymers ⓘ

There are no such residues in this entry.