



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 01:39 PM GMT

PDB ID : 2BXE
Title : Human serum albumin complexed with diflunisal
Authors : Ghuman, J.; Zunszain, P.A.; Petitpas, I.; Bhattacharya, A.A.; Curry, S.
Deposited on : 2005-07-26
Resolution : 2.95 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

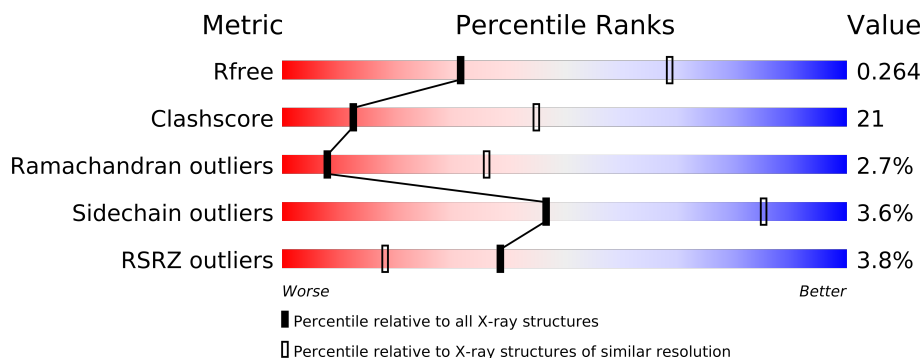
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.95 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}	66092	1587 (3.00-2.92)
Clashscore	79885	2029 (3.00-2.92)
Ramachandran outliers	78287	1955 (3.00-2.92)
Sidechain outliers	78261	1958 (3.00-2.92)
RSRZ outliers	66119	1588 (3.00-2.92)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	585	
1	B	585	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	1FL	A	2003	-	X
2	1FL	B	2002	-	X
2	1FL	B	2003	-	X

2 Entry composition i

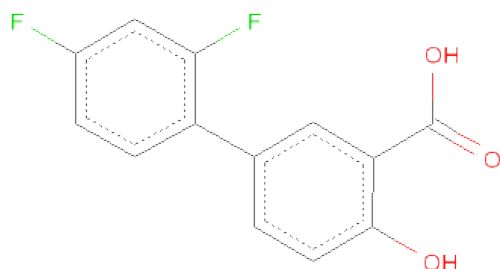
There are 2 unique types of molecules in this entry. The entry contains 8710 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called SERUM ALBUMIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	569	Total	C	N	O	S	0	0	0
			4344	2743	722	839	40			
1	B	566	Total	C	N	O	S	0	0	0
			4258	2692	710	816	40			

- Molecule 2 is 5-(2,4-DIFLUOROPHENYL)-2-HYDROXY-BENZOICACID (three-letter code: 1FL) (formula: C₁₃H₈F₂O₃).

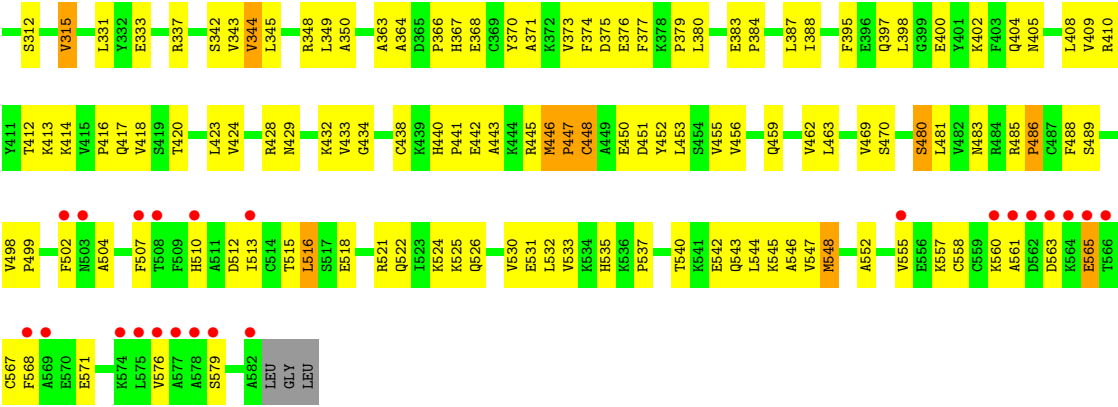


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	F	O	0	0
			18	13	2	3		
2	A	1	Total	C	F	O	0	0
			18	13	2	3		
2	A	1	Total	C	F	O	0	0
			18	13	2	3		
2	B	1	Total	C	F	O	0	0
			18	13	2	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	F	O	0	0
			18	13	2	3		
2	B	1	Total	C	F	O	0	0
			18	13	2	3		



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	55.41Å 55.53Å 120.52Å 81.54° 90.09° 65.93°	Depositor
Resolution (Å)	38.22 – 2.95 38.22 – 2.95	Depositor EDS
% Data completeness (in resolution range)	98.4 (38.22-2.95) 98.4 (38.22-2.95)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 2.95Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.226 , 0.270 0.222 , 0.264	Depositor DCC
R_{free} test set	1280 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	73.1	Xtriage
Anisotropy	0.328	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 54.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 27267 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8710	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.66% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 1FL

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	0.45	0/4428	0.66	0/6011
1	B	0.45	0/4339	0.65	0/5895
All	All	0.45	0/8767	0.65	0/11906

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4344	0	4056	159	0
1	B	4258	0	3962	193	0
2	A	54	0	18	3	0
2	B	54	0	18	7	0
All	All	8710	0	8054	352	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 21.

All (352) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:433:VAL:HG22	1:A:452:TYR:HD2	1.06	1.10
1:A:433:VAL:HG22	1:A:452:TYR:CD2	1.91	1.05
1:B:433:VAL:HG22	1:B:452:TYR:HD2	1.30	0.95
1:B:433:VAL:HG22	1:B:452:TYR:CD2	2.02	0.93
1:B:222:ARG:HD3	2:B:2003:1FL:FAE	1.59	0.91
1:B:120:VAL:HG21	1:B:175:ALA:HA	1.53	0.88
1:A:222:ARG:HD3	2:A:2003:1FL:FAE	1.63	0.88
1:A:151:ALA:HB3	1:A:152:PRO:HD3	1.55	0.87
1:B:364:ALA:O	1:B:366:PRO:HD3	1.75	0.87
1:B:95:GLU:OE1	1:B:99:ASN:HB2	1.74	0.85
1:B:57:GLU:HG3	1:B:58:SER:H	1.42	0.85
1:B:567:CYS:SG	1:B:571:GLU:HB2	2.16	0.85
1:B:151:ALA:HB3	1:B:152:PRO:HD3	1.56	0.85
1:A:276:LYS:HD2	1:A:277:GLU:H	1.42	0.83
1:A:222:ARG:HG3	1:A:295:ASN:OD1	1.79	0.82
1:B:540:THR:HG23	1:B:543:GLN:H	1.42	0.81
1:A:120:VAL:HG11	1:A:174:LYS:HB2	1.61	0.81
1:B:222:ARG:HG3	1:B:295:ASN:OD1	1.79	0.81
1:A:417:GLN:OE1	1:A:417:GLN:N	2.13	0.80
1:B:383:GLU:HB3	1:B:384:PRO:HD3	1.60	0.80
1:A:424:VAL:O	1:A:428:ARG:HG3	1.82	0.80
1:A:135:LEU:HD11	1:A:162:LYS:HG3	1.64	0.79
1:A:390:GLN:O	1:A:393:GLU:N	2.13	0.79
1:B:281:LYS:HD2	1:B:285:GLU:HG2	1.65	0.79
1:A:383:GLU:HB3	1:A:384:PRO:HD3	1.66	0.78
1:A:550:ASP:O	1:A:554:PHE:HD1	1.66	0.78
1:A:182:LEU:O	1:A:186:ARG:HG2	1.84	0.78
1:A:547:VAL:HG12	1:A:551:PHE:HE1	1.46	0.77
1:B:345:LEU:HD22	1:B:446:MET:CE	2.15	0.77
1:A:61:ASN:HD22	1:A:64:LYS:HE3	1.50	0.77
1:B:446:MET:HB3	1:B:447:PRO:HD3	1.69	0.75
1:B:59:ALA:HB3	1:B:62:CYS:SG	2.27	0.74
1:A:107:ASP:OD2	1:A:110:PRO:HA	1.87	0.74
1:B:265:CYS:O	1:B:268:GLN:HG3	1.88	0.74
1:A:547:VAL:CG1	1:A:551:PHE:HE1	2.00	0.74
1:B:110:PRO:HB2	1:B:112:LEU:CD2	2.17	0.74
1:A:169:CYS:HA	1:A:174:LYS:HD3	1.71	0.73
1:A:414:LYS:O	1:A:472:ARG:NH1	2.23	0.72
1:B:127:PHE:O	1:B:131:GLU:HB3	1.91	0.71
1:B:106:LYS:HD3	1:B:147:PRO:HB2	1.71	0.71
1:A:485:ARG:HB3	1:A:486:PRO:HD3	1.73	0.70
1:A:376:GLU:O	1:A:379:PRO:HD2	1.91	0.70
1:A:373:VAL:HG13	1:A:374:PHE:HD1	1.55	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:499:PRO:HB3	1:B:535:HIS:O	1.89	0.70
1:A:400:GLU:O	1:A:404:GLN:HG3	1.91	0.70
1:A:120:VAL:HG21	1:A:175:ALA:HA	1.75	0.69
1:B:194:ALA:HB1	1:B:455:VAL:CG1	2.22	0.69
1:B:214:TRP:CD1	1:B:343:VAL:HG11	2.27	0.69
1:B:285:GLU:O	1:B:289:CYS:HB2	1.93	0.69
1:B:561:ALA:HB3	1:B:563:ASP:OD1	1.93	0.69
1:B:483:ASN:O	1:B:486:PRO:HD2	1.92	0.68
1:B:206:PHE:CD2	1:B:481:LEU:HD22	2.29	0.68
1:A:276:LYS:CD	1:A:277:GLU:H	2.06	0.68
1:B:510:HIS:HA	1:B:568:PHE:CD2	2.28	0.68
1:A:151:ALA:HB3	1:A:152:PRO:CD	2.24	0.68
1:B:485:ARG:HB3	1:B:486:PRO:HD3	1.76	0.68
1:A:281:LYS:HB2	1:A:282:PRO:CD	2.25	0.67
1:B:260:LEU:O	1:B:260:LEU:HD23	1.94	0.67
1:B:32:GLN:NE2	1:B:110:PRO:HG2	2.10	0.67
1:A:35:PRO:HD2	1:A:38:ASP:OD2	1.95	0.67
1:A:305:LEU:HD21	1:A:333:GLU:HB3	1.77	0.66
1:B:110:PRO:HB2	1:B:112:LEU:HD22	1.76	0.66
1:B:10:ARG:O	1:B:14:LEU:HD23	1.95	0.66
1:B:344:VAL:HG22	1:B:451:ASP:OD1	1.96	0.65
1:B:565:GLU:O	1:B:568:PHE:HB3	1.96	0.65
1:A:66:LEU:O	1:A:70:PHE:HD1	1.78	0.65
1:B:290:ILE:O	1:B:293:VAL:HG12	1.98	0.64
1:A:483:ASN:O	1:A:486:PRO:HD2	1.98	0.64
1:A:276:LYS:HD3	1:A:277:GLU:HG2	1.81	0.63
1:A:529:LEU:HD22	1:A:548:MET:CE	2.28	0.63
1:A:214:TRP:CD1	1:A:343:VAL:HG11	2.33	0.63
1:B:66:LEU:O	1:B:70:PHE:HD1	1.82	0.63
1:B:400:GLU:O	1:B:404:GLN:HG3	1.97	0.62
1:B:441:PRO:O	1:B:443:ALA:N	2.31	0.62
1:B:151:ALA:HB3	1:B:152:PRO:CD	2.28	0.62
1:A:198:LEU:HD22	1:A:455:VAL:HA	1.82	0.61
1:B:558:CYS:SG	1:B:571:GLU:HB3	2.40	0.61
1:A:240:LYS:O	1:A:244:GLU:HG3	2.01	0.61
1:A:281:LYS:HB2	1:A:282:PRO:HD2	1.82	0.61
1:B:9:HIS:CD2	1:B:13:ASP:OD2	2.54	0.60
1:B:116:VAL:O	1:B:118:PRO:HD3	2.01	0.60
1:A:408:LEU:HD11	1:A:526:GLN:HB3	1.83	0.60
1:A:224:PRO:HB2	1:A:299:PRO:HD3	1.83	0.60
1:A:519:LYS:O	1:A:523:ILE:HG13	2.02	0.60
1:B:42:LEU:O	1:B:46:VAL:HG23	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:150:TYR:OH	2:A:2003:1FL:OAD	2.19	0.59
1:B:263:TYR:C	1:B:263:TYR:CD2	2.75	0.59
1:A:426:VAL:O	1:A:430:LEU:HG	2.03	0.59
1:B:441:PRO:C	1:B:443:ALA:H	2.04	0.59
1:B:32:GLN:HE22	1:B:110:PRO:CG	2.16	0.59
1:B:179:LEU:HB2	1:B:180:PRO:HD3	1.85	0.59
1:A:373:VAL:HG13	1:A:374:PHE:CD1	2.38	0.58
1:B:29:GLN:HG2	1:B:143:ALA:O	2.03	0.58
1:B:510:HIS:HA	1:B:568:PHE:HD2	1.66	0.58
1:B:120:VAL:HG21	1:B:175:ALA:CA	2.31	0.58
1:A:378:LYS:HB3	1:A:379:PRO:HD3	1.86	0.58
1:B:57:GLU:OE1	1:B:57:GLU:HA	2.03	0.58
1:B:513:ILE:HD12	1:B:555:VAL:HG23	1.85	0.57
1:A:450:GLU:HG3	1:A:450:GLU:O	2.03	0.57
1:B:417:GLN:H	1:B:417:GLN:CD	2.07	0.57
1:B:424:VAL:O	1:B:428:ARG:HG3	2.04	0.57
1:B:518:GLU:O	1:B:522:GLN:HG3	2.04	0.57
1:B:420:THR:HG23	1:B:530:VAL:HG11	1.87	0.57
1:A:510:HIS:HA	1:A:568:PHE:CB	2.35	0.57
1:B:532:LEU:HD21	1:B:547:VAL:HG11	1.87	0.57
1:B:27:PHE:CD2	1:B:74:LEU:HD21	2.40	0.56
1:B:32:GLN:NE2	1:B:110:PRO:CG	2.67	0.56
1:B:424:VAL:HG23	1:B:530:VAL:HG21	1.86	0.56
1:B:117:ARG:NH2	1:B:182:LEU:HB3	2.19	0.56
1:A:345:LEU:HD23	1:A:446:MET:CE	2.35	0.56
1:A:194:ALA:HB1	1:A:455:VAL:CG1	2.36	0.56
1:B:348:ARG:NH2	1:B:450:GLU:OE2	2.30	0.56
1:B:405:ASN:O	1:B:409:VAL:HG23	2.04	0.56
1:A:5:SER:HA	1:A:62:CYS:O	2.05	0.56
1:B:502:PHE:HE2	1:B:507:PHE:HB2	1.70	0.56
1:B:376:GLU:O	1:B:379:PRO:HD2	2.06	0.56
1:B:543:GLN:O	1:B:546:ALA:HB3	2.06	0.55
1:B:513:ILE:CD1	1:B:555:VAL:HG23	2.36	0.55
1:B:107:ASP:HB3	1:B:110:PRO:HG3	1.87	0.55
1:B:260:LEU:HD22	2:B:2003:1FL:HAR	1.87	0.55
1:B:441:PRO:C	1:B:443:ALA:N	2.58	0.55
1:B:408:LEU:HD11	1:B:526:GLN:HB3	1.89	0.55
1:B:151:ALA:CB	1:B:152:PRO:HD3	2.35	0.55
1:B:168:CYS:SG	1:B:177:CYS:C	2.84	0.55
1:B:446:MET:CB	1:B:447:PRO:HD3	2.37	0.55
1:A:325:VAL:O	1:A:329:MET:HG3	2.07	0.55
1:B:558:CYS:SG	1:B:571:GLU:CB	2.95	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:550:ASP:O	1:A:554:PHE:CD1	2.55	0.54
1:A:8:ALA:O	1:A:12:LYS:HG2	2.07	0.54
1:B:502:PHE:CE2	1:B:507:PHE:HB2	2.42	0.54
1:A:14:LEU:HD13	1:A:22:LEU:HD12	1.90	0.54
1:B:305:LEU:HD21	1:B:333:GLU:HB3	1.90	0.54
1:B:57:GLU:O	1:B:58:SER:C	2.46	0.54
1:A:380:LEU:O	1:A:384:PRO:HD2	2.08	0.53
1:A:222:ARG:C	1:A:224:PRO:HD3	2.29	0.53
1:A:547:VAL:CG1	1:A:551:PHE:CE1	2.88	0.53
1:B:117:ARG:HH22	1:B:182:LEU:HB3	1.73	0.53
1:A:276:LYS:CD	1:A:277:GLU:HG2	2.38	0.53
1:B:345:LEU:HD22	1:B:446:MET:HE1	1.89	0.53
1:A:89:ASP:O	1:A:92:ALA:HB3	2.09	0.53
1:A:331:LEU:HD13	1:A:350:ALA:HB2	1.90	0.53
1:B:331:LEU:HD13	1:B:350:ALA:HB2	1.91	0.53
1:A:522:GLN:O	1:A:526:GLN:HG3	2.09	0.53
1:B:567:CYS:SG	1:B:571:GLU:CB	2.95	0.53
1:A:179:LEU:HB2	1:A:180:PRO:HD3	1.90	0.52
1:B:516:LEU:H	1:B:516:LEU:HD12	1.74	0.52
1:B:115:LEU:HG	1:B:145:ARG:CZ	2.39	0.52
1:B:32:GLN:HE22	1:B:110:PRO:HG3	1.74	0.52
1:B:480:SER:OG	1:B:483:ASN:HB2	2.09	0.52
1:B:440:HIS:HB3	1:B:441:PRO:CD	2.39	0.52
1:A:279:CYS:HA	1:A:286:LYS:CD	2.40	0.52
1:A:49:PHE:O	1:A:49:PHE:HD2	1.93	0.52
1:A:464:HIS:HE1	1:A:470:SER:H	1.58	0.52
1:B:540:THR:HG22	1:B:543:GLN:HB2	1.91	0.52
1:A:224:PRO:HD2	1:A:296:ASP:HB3	1.92	0.51
1:A:151:ALA:CB	1:A:152:PRO:HD3	2.36	0.51
1:A:480:SER:OG	1:A:483:ASN:HB2	2.10	0.51
1:B:25:ILE:O	1:B:29:GLN:HG3	2.10	0.51
1:A:342:SER:HB2	1:A:451:ASP:OD2	2.10	0.51
1:A:161:TYR:O	1:A:164:ALA:HB3	2.11	0.51
1:B:26:ALA:HB2	1:B:250:LEU:HD12	1.92	0.51
1:B:432:LYS:O	1:B:433:VAL:C	2.47	0.51
1:A:9:HIS:C	1:A:9:HIS:HD1	2.14	0.51
1:A:383:GLU:HB3	1:A:384:PRO:CD	2.40	0.51
1:B:237:ASP:CB	1:B:260:LEU:HD12	2.41	0.51
1:B:51:LYS:HA	1:B:54:VAL:HG23	1.92	0.50
1:B:418:VAL:CG1	1:B:423:LEU:HG	2.41	0.50
1:B:408:LEU:O	1:B:412:THR:OG1	2.20	0.50
1:A:531:GLU:HA	1:A:531:GLU:OE1	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:464:HIS:CE1	1:A:469:VAL:H	2.30	0.50
1:A:343:VAL:O	1:A:347:LEU:HG	2.12	0.50
1:B:456:VAL:O	1:B:459:GLN:N	2.42	0.50
1:B:535:HIS:O	1:B:537:PRO:HD3	2.11	0.50
1:B:36:PHE:O	1:B:40:VAL:HG23	2.11	0.50
1:A:420:THR:O	1:A:424:VAL:HG23	2.11	0.50
1:B:409:VAL:O	1:B:413:LYS:HG3	2.12	0.49
1:B:150:TYR:HB2	1:B:196:GLN:HG2	1.94	0.49
1:A:345:LEU:HD23	1:A:446:MET:HE1	1.94	0.49
1:B:224:PRO:HD2	1:B:296:ASP:HB3	1.95	0.49
1:A:186:ARG:O	1:A:190:LYS:HG3	2.12	0.49
1:B:535:HIS:C	1:B:537:PRO:HD3	2.31	0.49
1:B:384:PRO:O	1:B:388:ILE:HG12	2.13	0.49
1:A:447:PRO:O	1:A:448:CYS:C	2.50	0.49
1:B:373:VAL:HG13	1:B:374:PHE:HD1	1.76	0.49
1:A:42:LEU:O	1:A:46:VAL:HG23	2.12	0.49
1:B:100:GLU:HG2	1:B:103:LEU:HD12	1.93	0.49
1:B:222:ARG:HA	1:B:295:ASN:OD1	2.13	0.49
1:A:417:GLN:CD	1:A:417:GLN:H	2.08	0.49
1:A:49:PHE:O	1:A:49:PHE:CD2	2.66	0.49
1:B:552:ALA:O	1:B:555:VAL:HG12	2.13	0.49
1:A:551:PHE:O	1:A:552:ALA:C	2.50	0.48
1:B:408:LEU:HD22	1:B:530:VAL:HG22	1.95	0.48
1:A:512:ASP:O	1:A:515:THR:HG22	2.14	0.48
1:A:155:LEU:O	1:A:158:ALA:HB3	2.13	0.48
1:B:417:GLN:N	1:B:417:GLN:CD	2.66	0.48
1:B:576:VAL:HA	1:B:579:SER:HB2	1.94	0.48
1:B:66:LEU:O	1:B:70:PHE:CD1	2.64	0.48
1:A:279:CYS:HA	1:A:286:LYS:HD2	1.96	0.48
1:A:342:SER:HB3	1:A:447:PRO:HA	1.94	0.48
1:B:481:LEU:N	2:B:2002:1FL:OAB	2.42	0.48
1:B:498:VAL:O	1:B:498:VAL:HG23	2.14	0.48
1:A:165:PHE:CE1	1:A:178:LEU:HD21	2.48	0.48
1:A:388:ILE:O	1:A:389:LYS:C	2.52	0.48
1:B:453:LEU:HD22	2:B:2001:1FL:HAQ	1.96	0.48
1:A:27:PHE:CE2	1:A:70:PHE:HD2	2.32	0.47
1:B:237:ASP:HB3	1:B:260:LEU:HD12	1.96	0.47
1:B:342:SER:HB3	1:B:447:PRO:HA	1.95	0.47
1:B:483:ASN:O	1:B:486:PRO:CD	2.62	0.47
1:B:274:LYS:CE	1:B:296:ASP:HA	2.44	0.47
1:A:275:LEU:HD23	1:A:293:VAL:HG11	1.96	0.47
1:A:26:ALA:HB2	1:A:250:LEU:HD12	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:66:LEU:O	1:A:70:PHE:CD1	2.65	0.47
1:A:141:GLU:OE1	1:A:144:ARG:HD3	2.14	0.47
1:A:168:CYS:SG	1:A:177:CYS:C	2.93	0.47
1:A:218:ARG:HD3	1:A:343:VAL:HG21	1.97	0.47
1:B:542:GLU:OE1	1:B:542:GLU:HA	2.14	0.47
1:A:550:ASP:O	1:A:553:ALA:HB3	2.15	0.47
1:B:453:LEU:CD2	2:B:2001:1FL:HAQ	2.44	0.47
1:B:260:LEU:C	1:B:260:LEU:HD23	2.35	0.47
1:B:540:THR:HG22	1:B:543:GLN:CG	2.45	0.47
1:B:9:HIS:HD2	1:B:13:ASP:OD2	1.96	0.47
1:A:532:LEU:O	1:A:535:HIS:HB3	2.15	0.47
1:A:32:GLN:HG2	1:A:144:ARG:O	2.15	0.47
1:B:521:ARG:O	1:B:525:LYS:HG3	2.15	0.46
1:B:384:PRO:HB2	1:B:446:MET:SD	2.55	0.46
1:A:88:ALA:O	1:A:89:ASP:C	2.53	0.46
1:A:348:ARG:HG3	1:A:482:VAL:HG12	1.96	0.46
1:B:151:ALA:CB	1:B:152:PRO:CD	2.93	0.46
1:B:398:LEU:HB3	1:B:402:LYS:HB2	1.96	0.46
1:B:138:TYR:O	1:B:142:ILE:HG12	2.14	0.46
1:A:390:GLN:O	1:A:392:CYS:N	2.49	0.46
1:A:206:PHE:CZ	1:A:481:LEU:HB2	2.51	0.46
1:A:420:THR:HB	1:A:421:PRO:HD3	1.97	0.46
1:B:312:SER:O	1:B:315:VAL:HG23	2.16	0.46
1:B:223:PHE:CD1	1:B:272:SER:HB2	2.51	0.45
1:A:127:PHE:CE1	1:A:131:GLU:HG3	2.51	0.45
1:A:265:CYS:O	1:A:268:GLN:HG3	2.15	0.45
1:B:522:GLN:HA	1:B:525:LYS:HD3	1.98	0.45
1:A:555:VAL:O	1:A:559:CYS:HB2	2.16	0.45
1:B:462:VAL:HG23	1:B:463:LEU:N	2.32	0.45
1:A:206:PHE:CE2	1:A:481:LEU:HB2	2.50	0.45
1:B:292:GLU:HG2	1:B:292:GLU:O	2.17	0.45
1:A:61:ASN:ND2	1:A:64:LYS:HE3	2.27	0.45
1:B:521:ARG:O	1:B:524:LYS:HB2	2.16	0.45
1:A:420:THR:CG2	1:A:527:THR:HG23	2.47	0.45
1:A:456:VAL:O	1:A:459:GLN:N	2.50	0.45
1:A:21:ALA:HB1	1:A:155:LEU:HD21	1.99	0.45
1:B:429:ASN:O	1:B:432:LYS:HB2	2.17	0.45
1:A:305:LEU:CD2	1:A:333:GLU:HB3	2.46	0.45
1:B:485:ARG:HE	1:B:485:ARG:HB3	1.63	0.45
1:A:66:LEU:HD22	1:A:70:PHE:HE1	1.82	0.45
1:A:513:ILE:HD11	1:A:555:VAL:HG13	1.99	0.45
1:A:520:GLU:O	1:A:524:LYS:HG3	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:19:PHE:O	1:B:23:VAL:HG23	2.17	0.45
1:B:150:TYR:OH	2:B:2003:1FL:OAB	2.22	0.44
1:A:500:LYS:O	1:A:535:HIS:ND1	2.47	0.44
1:A:532:LEU:HD11	1:A:547:VAL:HG11	1.99	0.44
1:A:49:PHE:CD2	1:A:49:PHE:C	2.88	0.44
1:A:290:ILE:HA	1:A:293:VAL:HG13	1.99	0.44
1:A:511:ALA:O	1:A:514:CYS:SG	2.76	0.44
1:B:274:LYS:HE2	1:B:296:ASP:HA	1.98	0.44
1:A:405:ASN:O	1:A:408:LEU:HB2	2.17	0.44
1:B:533:VAL:CG2	1:B:544:LEU:HD21	2.48	0.44
1:B:558:CYS:C	1:B:560:LYS:H	2.20	0.44
1:B:16:GLU:O	1:B:20:LYS:HG3	2.18	0.44
1:A:521:ARG:O	1:A:524:LYS:N	2.48	0.44
1:B:274:LYS:HD2	1:B:294:GLU:OE2	2.18	0.44
1:A:441:PRO:O	1:A:442:GLU:C	2.56	0.44
1:A:30:TYR:CD1	1:A:102:PHE:HB3	2.53	0.44
1:B:14:LEU:N	1:B:14:LEU:HD22	2.33	0.44
1:B:286:LYS:O	1:B:289:CYS:HB3	2.18	0.44
1:A:216:VAL:HG22	1:A:235:VAL:HG21	2.00	0.44
1:A:278:CYS:O	1:A:281:LYS:HG2	2.18	0.43
1:A:34:CYS:HA	1:A:35:PRO:HD3	1.88	0.43
1:B:383:GLU:HB3	1:B:384:PRO:CD	2.41	0.43
1:B:502:PHE:CZ	1:B:504:ALA:HA	2.54	0.43
1:A:567:CYS:O	1:A:571:GLU:N	2.46	0.43
1:B:483:ASN:C	1:B:486:PRO:HD2	2.38	0.43
1:A:141:GLU:OE1	1:A:141:GLU:HA	2.17	0.43
1:A:257:ARG:HG2	1:A:257:ARG:O	2.18	0.43
1:B:161:TYR:O	1:B:164:ALA:HB3	2.17	0.43
1:A:458:ASN:O	1:A:462:VAL:HG22	2.18	0.43
1:B:567:CYS:O	1:B:571:GLU:N	2.50	0.43
1:A:120:VAL:HG21	1:A:175:ALA:CA	2.45	0.43
1:B:533:VAL:HG22	1:B:544:LEU:HD21	2.01	0.43
1:B:557:LYS:HB3	1:B:571:GLU:OE2	2.18	0.43
1:B:558:CYS:C	1:B:560:LYS:N	2.71	0.43
1:B:110:PRO:HB2	1:B:112:LEU:HD21	1.97	0.43
1:A:68:THR:O	1:A:72:ASP:OD2	2.37	0.43
1:B:414:LYS:HE3	1:B:488:PHE:O	2.19	0.43
1:B:433:VAL:O	1:B:434:GLY:C	2.54	0.43
1:A:206:PHE:CE2	1:A:481:LEU:HD13	2.54	0.43
1:A:112:LEU:HA	1:A:113:PRO:HD3	1.91	0.43
1:B:194:ALA:HB1	1:B:455:VAL:HG13	2.01	0.42
1:B:209:ARG:HH21	2:B:2002:1FL:HAH	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:447:PRO:O	1:B:448:CYS:C	2.57	0.42
1:B:410:ARG:O	1:B:414:LYS:HG3	2.20	0.42
1:B:417:GLN:OE1	1:B:417:GLN:N	2.35	0.42
1:B:333:GLU:O	1:B:337:ARG:HG3	2.19	0.42
1:B:51:LYS:C	1:B:53:CYS:H	2.23	0.42
1:B:272:SER:HB3	1:B:275:LEU:HG	2.01	0.42
1:B:531:GLU:OE1	1:B:531:GLU:HA	2.19	0.42
1:A:483:ASN:O	1:A:486:PRO:CD	2.64	0.42
1:A:432:LYS:O	1:A:433:VAL:C	2.56	0.42
1:B:89:ASP:O	1:B:92:ALA:HB3	2.18	0.42
1:B:434:GLY:HA2	1:B:438:CYS:SG	2.60	0.42
1:A:345:LEU:HD23	1:A:446:MET:HE3	2.02	0.42
1:A:48:GLU:O	1:A:52:THR:HG23	2.20	0.42
1:A:25:ILE:HD13	1:A:154:LEU:HD23	2.01	0.42
1:B:563:ASP:OD2	1:B:567:CYS:N	2.50	0.41
1:B:107:ASP:O	1:B:110:PRO:HG3	2.20	0.41
1:A:464:HIS:CE1	1:A:470:SER:H	2.36	0.41
1:B:367:HIS:O	1:B:371:ALA:HB2	2.19	0.41
1:A:109:ASN:HD22	1:A:109:ASN:HA	1.62	0.41
1:B:540:THR:CG2	1:B:543:GLN:HB2	2.50	0.41
1:A:384:PRO:HB2	1:A:446:MET:SD	2.60	0.41
1:B:293:VAL:HG22	1:B:294:GLU:N	2.34	0.41
1:B:512:ASP:O	1:B:515:THR:HG22	2.21	0.41
1:B:117:ARG:HG3	1:B:117:ARG:O	2.21	0.41
1:B:545:LYS:HA	1:B:548:MET:HB2	2.01	0.41
1:B:540:THR:CG2	1:B:543:GLN:HG3	2.51	0.41
1:A:120:VAL:CG1	1:A:174:LYS:HB2	2.41	0.41
1:A:373:VAL:O	1:A:376:GLU:HB2	2.21	0.41
1:A:290:ILE:O	1:A:293:VAL:HG22	2.21	0.41
1:B:107:ASP:OD2	1:B:110:PRO:HA	2.20	0.41
1:B:417:GLN:HB2	1:B:470:SER:HB2	2.03	0.41
1:B:349:LEU:HD22	1:B:377:PHE:CG	2.55	0.41
1:B:24:LEU:HD13	1:B:43:VAL:HG21	2.01	0.41
1:A:395:PHE:O	1:A:397:GLN:N	2.54	0.41
1:B:237:ASP:HB2	1:B:260:LEU:HD12	2.02	0.41
1:A:274:LYS:HA	1:A:276:LYS:HE3	2.02	0.41
1:B:32:GLN:NE2	1:B:144:ARG:O	2.45	0.41
1:B:412:THR:O	1:B:416:PRO:HG3	2.21	0.41
1:A:158:ALA:O	1:A:161:TYR:HB3	2.21	0.41
1:B:459:GLN:O	1:B:462:VAL:HG22	2.21	0.41
1:B:395:PHE:C	1:B:397:GLN:N	2.74	0.41
1:B:238:LEU:HA	1:B:238:LEU:HD12	1.87	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:453:LEU:CD2	2:A:2001:1FL:HAQ	2.51	0.41
1:A:262:LYS:O	1:A:263:TYR:C	2.59	0.41
1:A:310:VAL:HG11	1:A:374:PHE:CE1	2.56	0.40
1:B:441:PRO:O	1:B:445:ARG:HG3	2.21	0.40
1:B:408:LEU:HD22	1:B:530:VAL:CG2	2.51	0.40
1:B:370:TYR:C	1:B:370:TYR:CD1	2.95	0.40
1:B:380:LEU:O	1:B:384:PRO:CD	2.68	0.40
1:A:410:ARG:O	1:A:414:LYS:HG3	2.22	0.40
1:A:72:ASP:O	1:A:76:THR:HG23	2.20	0.40
1:B:61:ASN:HD22	1:B:64:LYS:CD	2.35	0.40
1:A:311:GLU:O	1:A:312:SER:C	2.59	0.40
1:A:359:LYS:HG3	1:A:360:CYS:N	2.36	0.40
1:B:446:MET:CB	1:B:447:PRO:CD	2.99	0.40
1:A:408:LEU:HD22	1:A:530:VAL:HG22	2.03	0.40
1:A:566:THR:C	1:A:568:PHE:N	2.73	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	565/585 (97%)	486 (86%)	65 (12%)	14 (2%)	9	38
1	B	562/585 (96%)	478 (85%)	68 (12%)	16 (3%)	8	34
All	All	1127/1170 (96%)	964 (86%)	133 (12%)	30 (3%)	8	36

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	59	ALA
1	A	60	GLU
1	B	54	VAL
1	B	57	GLU
1	B	58	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	300	ALA
1	B	565	GLU
1	A	390	GLN
1	A	391	ASN
1	A	562	ASP
1	B	442	GLU
1	A	58	SER
1	A	312	SER
1	A	447	PRO
1	A	557	LYS
1	B	315	VAL
1	B	363	ALA
1	A	300	ALA
1	A	448	CYS
1	B	447	PRO
1	A	57	GLU
1	B	276	LYS
1	A	55	ALA
1	B	60	GLU
1	B	75	CYS
1	B	281	LYS
1	B	448	CYS
1	B	118	PRO
1	B	469	VAL
1	A	151	ALA

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	447/511 (88%)	432 (97%)	15 (3%)	49	86
1	B	432/511 (84%)	415 (96%)	17 (4%)	43	83
All	All	879/1022 (86%)	847 (96%)	32 (4%)	47	85

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

Mol	Chain	Res	Type
1	A	37	GLU
1	A	49	PHE
1	A	109	ASN
1	A	152	PRO
1	A	198	LEU
1	A	276	LYS
1	A	310	VAL
1	A	384	PRO
1	A	440	HIS
1	A	442	GLU
1	A	467	THR
1	A	480	SER
1	A	486	PRO
1	A	489	SER
1	A	532	LEU
1	B	111	ASN
1	B	152	PRO
1	B	167	GLU
1	B	182	LEU
1	B	209	ARG
1	B	245	CYS
1	B	263	TYR
1	B	344	VAL
1	B	368	GLU
1	B	375	ASP
1	B	387	LEU
1	B	446	MET
1	B	480	SER
1	B	486	PRO
1	B	489	SER
1	B	516	LEU
1	B	548	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	61	ASN
1	A	99	ASN
1	A	109	ASN
1	A	318	ASN
1	A	338	HIS
1	A	429	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	459	GLN
1	A	464	HIS
1	A	483	ASN
1	A	543	GLN
1	B	9	HIS
1	B	111	ASN
1	B	338	HIS
1	B	464	HIS
1	B	483	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

6 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	1FL	A	2001	-	19,19,19	1.31	2 (10%)	27,27,27	0.98	1 (3%)
2	1FL	A	2002	-	19,19,19	1.27	1 (5%)	27,27,27	1.13	1 (3%)
2	1FL	A	2003	-	19,19,19	0.57	0	27,27,27	0.86	0
2	1FL	B	2001	-	19,19,19	1.31	1 (5%)	27,27,27	0.96	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	1FL	B	2002	-	19,19,19	1.25	1 (5%)	27,27,27	1.11	2 (7%)
2	1FL	B	2003	-	19,19,19	1.23	2 (10%)	27,27,27	1.28	3 (11%)

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	1FL	A	2001	-	-	0/8/8/8	0/2/2/2
2	1FL	A	2002	-	-	0/8/8/8	0/2/2/2
2	1FL	A	2003	-	-	0/8/8/8	0/2/2/2
2	1FL	B	2001	-	-	0/8/8/8	0/2/2/2
2	1FL	B	2002	-	-	0/8/8/8	0/2/2/2
2	1FL	B	2003	-	-	0/8/8/8	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2001	1FL	CAO-CAN	3.77	1.43	1.39
2	A	2002	1FL	CAO-CAN	3.68	1.43	1.39
2	A	2001	1FL	CAO-CAN	3.63	1.43	1.39
2	B	2002	1FL	CAO-CAN	3.63	1.43	1.39
2	B	2003	1FL	CAH-CAO	3.17	1.45	1.40
2	B	2003	1FL	CAH-CAG	2.15	1.42	1.38
2	A	2001	1FL	CAM-CAN	2.04	1.41	1.37

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2002	1FL	FAT-CAN-CAO	3.12	123.28	118.79
2	B	2002	1FL	FAT-CAN-CAO	3.09	123.24	118.79
2	B	2003	1FL	CAN-CAM-CAF	2.74	119.64	116.66
2	B	2001	1FL	FAT-CAN-CAO	2.39	122.23	118.79
2	B	2003	1FL	CAH-CAG-CAF	-2.32	115.88	118.33
2	A	2001	1FL	FAT-CAN-CAO	2.31	122.12	118.79
2	B	2003	1FL	OAL-CAK-CAJ	2.14	125.70	121.69
2	B	2002	1FL	CAN-CAM-CAF	2.04	118.87	116.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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(Å ²)	Q<0.9
1	A	569/585 (97%)	-0.16	18 (3%)	45 20	35, 78, 156, 170	0
1	B	566/585 (96%)	-0.09	25 (4%)	33 16	35, 78, 148, 175	0
All	All	1135/1170 (97%)	-0.13	43 (3%)	38 18	35, 78, 150, 175	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	582	ALA	9.4
1	B	566	THR	7.3
1	B	579	SER	6.3
1	A	563	ASP	5.9
1	B	564	LYS	5.4
1	B	562	ASP	4.9
1	B	577	ALA	4.9
1	B	575	LEU	4.8
1	B	578	ALA	4.8
1	A	508	THR	4.5
1	B	513	ILE	3.8
1	A	569	ALA	3.5
1	B	568	PHE	3.5
1	A	579	SER	3.3
1	A	91	CYS	3.3
1	B	507	PHE	3.1
1	A	562	ASP	3.1
1	A	506	THR	3.1
1	A	513	ILE	3.0
1	A	138	TYR	2.9
1	A	560	LYS	2.9
1	B	510	HIS	2.9
1	B	508	THR	2.7
1	A	561	ALA	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	509	PHE	2.7
1	A	92	ALA	2.5
1	B	54	VAL	2.5
1	A	572	GLY	2.5
1	A	568	PHE	2.4
1	B	565	GLU	2.3
1	B	561	ALA	2.3
1	B	560	LYS	2.2
1	B	563	ASP	2.2
1	A	555	VAL	2.2
1	A	300	ALA	2.1
1	B	502	PHE	2.1
1	B	574	LYS	2.1
1	B	503	ASN	2.1
1	A	102	PHE	2.0
1	B	555	VAL	2.0
1	B	569	ALA	2.0
1	B	96	PRO	2.0
1	B	576	VAL	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	1FL	A	2003	18/18	0.30	5.01	109,109,111,111	0
2	1FL	B	2003	18/18	0.36	3.74	98,101,102,104	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	1FL	B	2002	18/18	0.34	3.68	91,94,99,100	0
2	1FL	B	2001	18/18	0.24	1.90	63,67,71,73	0
2	1FL	A	2002	18/18	0.25	1.73	77,82,91,92	0
2	1FL	A	2001	18/18	0.19	0.29	55,58,66,68	0

6.5 Other polymers ⓘ

There are no such residues in this entry.