Full wwPDB X-ray Structure Validation Report (i)

Dec 10, 2023 – 07:31 am GMT

PDB ID	:	2BXA
Title	:	Human serum albumin complexed with 3-carboxy-4-methyl-5-propyl-2-furanpropanoic acid (CMPF)
Authors	:	Ghuman, J.; Zunszain, P.A.; Petitpas, I.; Bhattacharya, A.A.; Otagiri, M.; Curry, S.
Deposited on	:	2005-07-26
Resolution	:	2.35 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 (i) 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 (i)) were used in the production of this report:

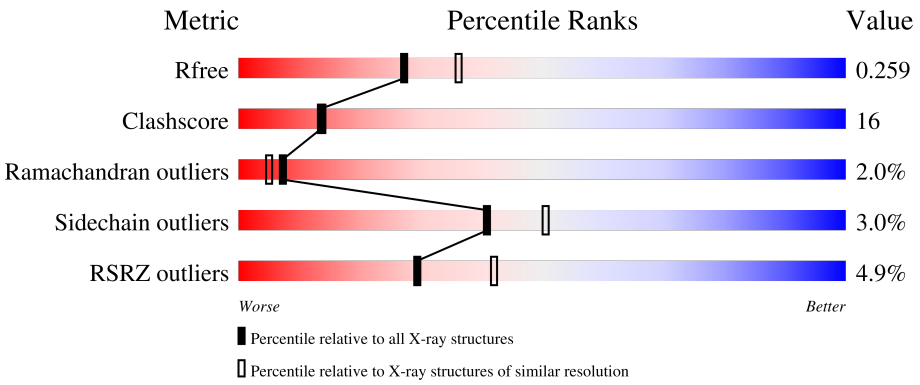
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.35 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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	585	4% 71% 25% • •
1	B	585	5% 65% 29% • •

2 Entry composition (i)

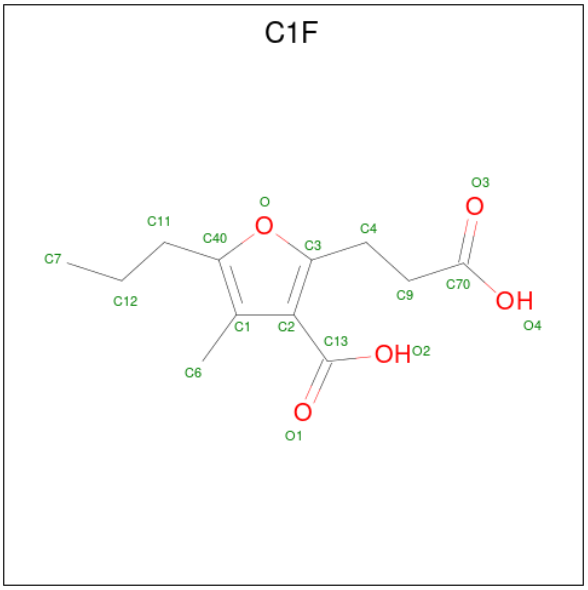
There are 2 unique types of molecules in this entry. The entry contains 8664 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	569	4341	2741	721	839	40	0	0	0
1	B	566	4255	2693	708	814	40	0	0	0

- Molecule 2 is 3-CARBOXY-4-METHYL-5-PROPYL-2-FURANPROPIONIC (three-letter code: C1F) (formula: $C_{12}H_{16}O_5$).



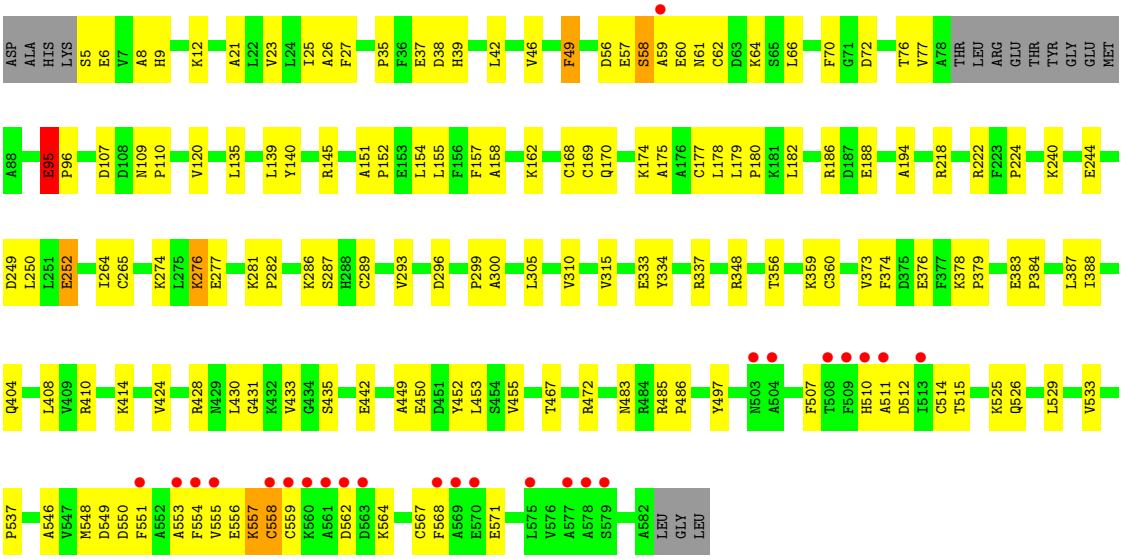
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	17	12	5	0	0
2	A	1	17	12	5	0	0
2	B	1	17	12	5	0	0
2	B	1	17	12	5	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

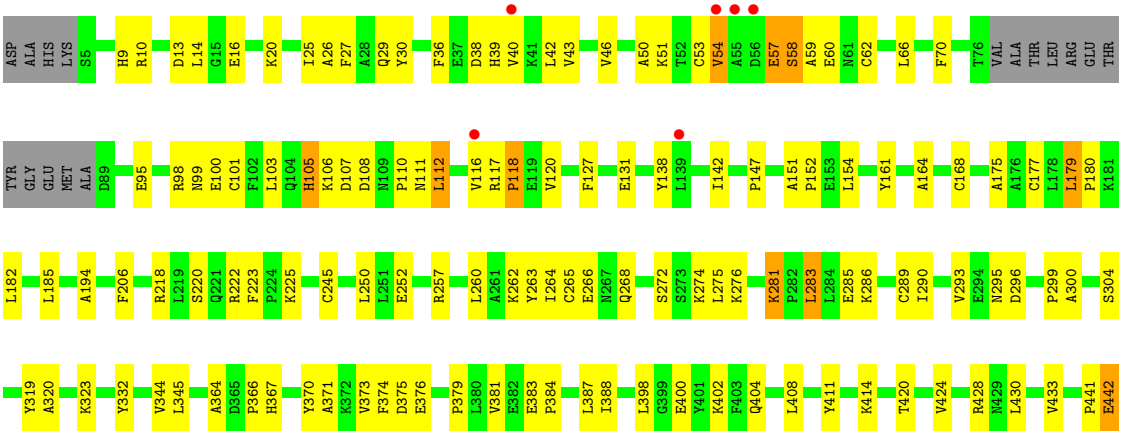
• Molecule 1: SERUM ALBUMIN

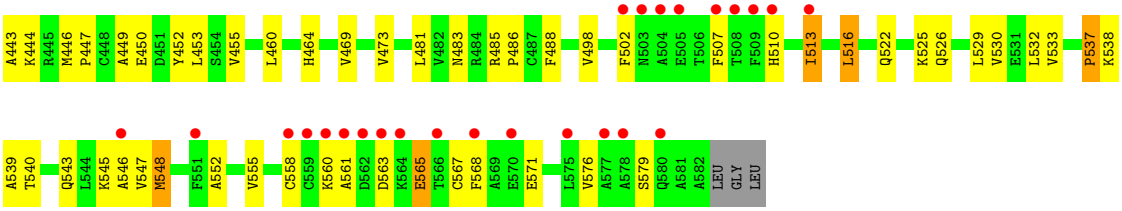
Chain A:



• Molecule 1: SERUM ALBUMIN

Chain B:




A443 K444 R445 M446 P447 C448 A449 E450 D451 Y452 L453 S454 V455 L460 H464 V469 V473 L481 V482 N483 R484 R485 P486 C487 F488 V498 F502 N503 A504 E505 T506 F507 T508 F509 H510 I513 L516 Q522 K525 Q526 L529 V530 E531 L532 V533 P537 K538
A539 T540 Q543 L544 K545 A546 V547 M548 F551 A552 V555 C558 C559 K560 A561 D562 D563 K564 E565 T566 C567 F568 A569 E570 E571 L575 V576 A577 A578 S579 Q580 A581 A582 LEU GLY LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	54.98Å 55.43Å 119.97Å 81.01° 90.88° 64.58°	Depositor
Resolution (Å)	49.20 – 2.35 49.24 – 2.35	Depositor EDS
% Data completeness (in resolution range)	95.3 (49.20-2.35) 95.5 (49.24-2.35)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.13 (at 2.34Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.230 , (Not available) 0.228 , 0.259	Depositor DCC
R_{free} test set	2505 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å^2)	47.2	Xtriage
Anisotropy	0.369	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 57.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8664	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.13% of the height of the origin peak. No significant pseudotranslation is detected.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: C1F

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	0.40	0/4425	0.59	1/6008 (0.0%)
1	B	0.37	0/4336	0.57	0/5890
All	All	0.39	0/8761	0.58	1/11898 (0.0%)

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	B	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	558	CYS	CA-CB-SG	5.11	123.20	114.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	411	TYR	Sidechain

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	4341	0	4047	118	0
1	B	4255	0	3964	149	0
2	A	34	0	28	5	0
2	B	34	0	28	2	0
All	All	8664	0	8067	267	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All (267) 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:95:GLU:HB3	1:A:96:PRO:HD3	1.16	1.12
1:B:516:LEU:HD12	1:B:516:LEU:H	1.12	1.09
1:A:95:GLU:HB3	1:A:96:PRO:CD	1.94	0.96
1:A:95:GLU:CB	1:A:96:PRO:HD3	1.95	0.96
1:A:218:ARG:NH2	1:A:222:ARG:HH21	1.64	0.96
1:B:433:VAL:HG22	1:B:452:TYR:CD2	2.05	0.92
1:B:120:VAL:HG21	1:B:175:ALA:HA	1.51	0.92
1:B:218:ARG:NH2	1:B:222:ARG:HH21	1.68	0.91
1:B:151:ALA:HB3	1:B:152:PRO:HD3	1.56	0.86
1:B:110:PRO:HB2	1:B:112:LEU:CD2	2.04	0.86
1:B:516:LEU:HD12	1:B:516:LEU:N	1.93	0.84
1:B:57:GLU:HG3	1:B:58:SER:H	1.40	0.84
1:B:66:LEU:O	1:B:70:PHE:HD1	1.62	0.82
1:A:151:ALA:HB3	1:A:152:PRO:HD3	1.62	0.81
1:A:135:LEU:HD11	1:A:162:LYS:HG3	1.64	0.80
1:A:424:VAL:O	1:A:428:ARG:HG3	1.82	0.79
1:B:95:GLU:OE1	1:B:99:ASN:HB2	1.82	0.79
1:B:424:VAL:O	1:B:428:ARG:HG3	1.83	0.78
1:A:383:GLU:HB3	1:A:384:PRO:HD3	1.67	0.77
1:B:218:ARG:HH21	1:B:222:ARG:HH21	1.33	0.77
1:B:433:VAL:HG22	1:B:452:TYR:HD2	1.48	0.76
1:B:364:ALA:O	1:B:366:PRO:HD3	1.84	0.76
1:A:120:VAL:HG11	1:A:174:LYS:HB2	1.67	0.75
1:A:169:CYS:HA	1:A:174:LYS:HD3	1.67	0.74
1:B:110:PRO:HB2	1:B:112:LEU:HD22	1.71	0.73
1:B:117:ARG:NH2	1:B:182:LEU:HB3	2.03	0.73
1:B:433:VAL:HG22	1:B:452:TYR:CE2	2.23	0.73
1:A:61:ASN:HD22	1:A:64:LYS:HE3	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:LEU:HB2	1:B:180:PRO:HD3	1.73	0.71
1:A:276:LYS:HD2	1:A:277:GLU:H	1.56	0.70
1:B:516:LEU:H	1:B:516:LEU:CD1	1.98	0.70
1:B:540:THR:HG23	1:B:543:GLN:H	1.56	0.70
1:A:276:LYS:CD	1:A:277:GLU:H	2.05	0.70
1:A:27:PHE:HE2	1:A:70:PHE:HD2	1.38	0.69
1:B:59:ALA:HB3	1:B:62:CYS:SG	2.32	0.69
1:B:281:LYS:HD2	1:B:285:GLU:HG2	1.73	0.69
1:A:120:VAL:HG21	1:A:175:ALA:HA	1.76	0.68
1:B:552:ALA:O	1:B:555:VAL:HG12	1.92	0.68
1:A:550:ASP:HB3	1:A:554:PHE:CZ	2.28	0.68
1:B:127:PHE:O	1:B:131:GLU:HB3	1.93	0.68
1:B:513:ILE:HA	1:B:516:LEU:HD11	1.74	0.68
1:A:378:LYS:HB3	1:A:379:PRO:HD3	1.74	0.68
1:B:117:ARG:HH22	1:B:182:LEU:HB3	1.56	0.68
1:A:27:PHE:CE2	1:A:70:PHE:HD2	2.13	0.67
1:B:345:LEU:HD22	1:B:446:MET:HE1	1.77	0.67
1:B:483:ASN:C	1:B:486:PRO:HD2	2.14	0.67
1:B:483:ASN:O	1:B:486:PRO:HD2	1.95	0.67
1:A:276:LYS:HD3	1:A:277:GLU:HG2	1.77	0.66
1:A:567:CYS:O	1:A:571:GLU:N	2.28	0.66
1:B:510:HIS:O	1:B:513:ILE:HG23	1.97	0.64
1:B:25:ILE:O	1:B:29:GLN:HG3	1.97	0.64
1:A:410:ARG:NH1	2:A:2002:C1F:H4C2	2.13	0.64
1:B:265:CYS:O	1:B:268:GLN:HG3	1.97	0.64
1:B:42:LEU:O	1:B:46:VAL:HG23	1.98	0.63
1:A:107:ASP:OD2	1:A:110:PRO:HA	1.98	0.63
1:A:218:ARG:HH21	1:A:222:ARG:HH21	1.47	0.62
1:B:9:HIS:CD2	1:B:13:ASP:OD2	2.53	0.62
1:A:182:LEU:O	1:A:186:ARG:HG2	2.00	0.61
1:B:120:VAL:HG21	1:B:175:ALA:CA	2.29	0.61
1:A:218:ARG:CZ	1:A:222:ARG:HH21	2.14	0.60
1:B:513:ILE:C	1:B:516:LEU:HD11	2.21	0.60
1:A:264:ILE:HD11	2:A:2001:C1F:H7C3	1.82	0.60
1:B:285:GLU:O	1:B:289:CYS:HB2	2.02	0.60
1:B:513:ILE:CA	1:B:516:LEU:HD11	2.32	0.59
1:A:373:VAL:HG13	1:A:374:PHE:HD1	1.68	0.59
1:A:408:LEU:HD11	1:A:526:GLN:HB3	1.83	0.59
1:B:430:LEU:O	1:B:433:VAL:HG23	2.02	0.59
1:A:8:ALA:O	1:A:12:LYS:HG2	2.02	0.59
1:B:281:LYS:HD2	1:B:285:GLU:OE2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:LYS:HB2	1:A:282:PRO:CD	2.33	0.59
1:A:551:PHE:HA	1:A:554:PHE:CD1	2.38	0.58
1:B:561:ALA:HB3	1:B:563:ASP:OD1	2.02	0.58
1:B:57:GLU:OE1	1:B:57:GLU:HA	2.03	0.58
1:A:240:LYS:O	1:A:244:GLU:HG3	2.03	0.58
1:A:179:LEU:HB2	1:A:180:PRO:HD3	1.85	0.58
1:A:281:LYS:HB2	1:A:282:PRO:HD2	1.86	0.57
1:B:283:LEU:O	1:B:286:LYS:HB3	2.04	0.57
1:A:35:PRO:HD2	1:A:38:ASP:OD2	2.04	0.57
1:A:265:CYS:SG	1:A:286:LYS:HD2	2.44	0.57
1:A:66:LEU:O	1:A:70:PHE:HD1	1.86	0.57
1:A:218:ARG:NH2	1:A:222:ARG:NH2	2.46	0.56
1:A:384:PRO:O	1:A:388:ILE:HG12	2.04	0.56
1:B:100:GLU:HG2	1:B:103:LEU:HD12	1.86	0.56
1:B:281:LYS:CD	1:B:285:GLU:OE2	2.53	0.56
1:B:116:VAL:O	1:B:118:PRO:HD3	2.06	0.56
1:B:384:PRO:O	1:B:388:ILE:HG12	2.06	0.56
1:A:359:LYS:HG3	1:A:360:CYS:N	2.21	0.56
1:B:319:TYR:O	1:B:323:LYS:HD3	2.06	0.56
1:B:262:LYS:O	1:B:266:GLU:HG3	2.07	0.55
1:A:157:PHE:HE2	1:A:188:GLU:HG2	1.70	0.55
1:A:546:ALA:O	1:A:550:ASP:OD1	2.23	0.55
1:B:502:PHE:HE2	1:B:507:PHE:HB2	1.71	0.55
1:A:135:LEU:HD11	1:A:162:LYS:CG	2.36	0.55
1:B:16:GLU:O	1:B:20:LYS:HG3	2.07	0.55
1:A:289:CYS:O	1:A:293:VAL:HG13	2.07	0.54
1:B:36:PHE:O	1:B:40:VAL:HG23	2.07	0.54
1:B:502:PHE:CE2	1:B:507:PHE:HB2	2.43	0.54
1:A:485:ARG:HB3	1:A:486:PRO:HD3	1.90	0.54
1:B:263:TYR:C	1:B:263:TYR:CD2	2.81	0.54
1:B:274:LYS:HE3	1:B:296:ASP:HA	1.88	0.54
1:B:565:GLU:O	1:B:568:PHE:HB3	2.08	0.54
1:B:383:GLU:HB3	1:B:384:PRO:HD3	1.89	0.53
1:A:95:GLU:CB	1:A:96:PRO:CD	2.68	0.53
1:B:373:VAL:HG13	1:B:374:PHE:HD1	1.74	0.53
1:B:510:HIS:HA	1:B:568:PHE:CD2	2.43	0.53
1:B:27:PHE:HE1	1:B:70:PHE:HD2	1.56	0.53
1:A:222:ARG:C	1:A:224:PRO:HD3	2.29	0.53
1:A:49:PHE:HD2	1:A:49:PHE:O	1.92	0.53
1:B:66:LEU:O	1:B:70:PHE:CD1	2.53	0.53
1:A:5:SER:HA	1:A:62:CYS:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:VAL:HG13	1:A:374:PHE:CD1	2.43	0.53
1:B:320:ALA:HA	1:B:323:LYS:HE2	1.91	0.53
1:B:194:ALA:HB1	1:B:455:VAL:CG1	2.39	0.53
1:B:400:GLU:O	1:B:404:GLN:HG3	2.08	0.53
1:A:525:LYS:HG2	1:A:551:PHE:CE2	2.44	0.53
1:A:157:PHE:CE2	1:A:188:GLU:HG2	2.45	0.52
1:A:178:LEU:HG	1:A:182:LEU:CD1	2.39	0.52
1:B:30:TYR:HE1	1:B:103:LEU:HD23	1.75	0.52
1:B:106:LYS:HD3	1:B:147:PRO:HB2	1.91	0.52
1:A:414:LYS:O	1:A:472:ARG:NH1	2.42	0.52
1:B:151:ALA:CB	1:B:152:PRO:HD3	2.35	0.52
1:A:224:PRO:HD2	1:A:296:ASP:HB3	1.90	0.52
1:B:110:PRO:HB2	1:B:112:LEU:HD21	1.87	0.52
1:B:168:CYS:SG	1:B:177:CYS:C	2.88	0.51
1:B:222:ARG:HG2	1:B:223:PHE:CE1	2.45	0.51
1:B:9:HIS:HD2	1:B:13:ASP:OD2	1.92	0.51
1:A:483:ASN:C	1:A:486:PRO:HD2	2.31	0.51
1:B:260:LEU:HD21	2:B:2001:C1F:H7C3	1.93	0.51
1:B:444:LYS:O	1:B:447:PRO:HD2	2.10	0.51
1:B:345:LEU:HD22	1:B:446:MET:CE	2.41	0.51
1:B:558:CYS:SG	1:B:571:GLU:CB	2.99	0.51
1:A:553:ALA:O	1:A:557:LYS:HG2	2.11	0.50
1:B:398:LEU:HB3	1:B:402:LYS:HB2	1.93	0.50
1:B:272:SER:HB3	1:B:275:LEU:HG	1.92	0.50
1:B:485:ARG:HB3	1:B:486:PRO:HD3	1.93	0.50
1:B:567:CYS:SG	1:B:571:GLU:HB2	2.52	0.50
1:B:27:PHE:CE1	1:B:70:PHE:HD2	2.29	0.50
1:A:139:LEU:HD21	1:A:158:ALA:HB2	1.92	0.50
1:A:168:CYS:SG	1:A:177:CYS:C	2.90	0.50
1:A:107:ASP:O	1:A:110:PRO:HD3	2.12	0.49
1:B:151:ALA:HB3	1:B:152:PRO:CD	2.36	0.49
1:A:305:LEU:HD21	1:A:333:GLU:HB3	1.93	0.49
1:B:453:LEU:HD11	2:B:2002:C1F:H121	1.93	0.49
1:B:222:ARG:HA	1:B:295:ASN:OD1	2.12	0.49
1:B:446:MET:HE3	1:B:450:GLU:OE1	2.12	0.49
1:B:441:PRO:O	1:B:443:ALA:N	2.46	0.49
1:A:252:GLU:H	1:A:252:GLU:CD	2.16	0.49
1:B:218:ARG:NH2	1:B:222:ARG:NH2	2.49	0.49
1:A:430:LEU:O	1:A:433:VAL:HG12	2.12	0.49
1:A:145:ARG:HG3	1:A:145:ARG:HH11	1.78	0.49
1:B:537:PRO:O	1:B:539:ALA:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:ILE:O	1:B:293:VAL:HG12	2.12	0.48
1:A:373:VAL:O	1:A:376:GLU:HB2	2.13	0.48
1:B:98:ARG:O	1:B:101:CYS:HB3	2.13	0.48
1:B:510:HIS:HA	1:B:568:PHE:HD2	1.76	0.48
1:A:224:PRO:HB2	1:A:299:PRO:HD3	1.96	0.48
1:B:286:LYS:O	1:B:290:ILE:HG13	2.13	0.48
1:A:483:ASN:O	1:A:486:PRO:HD2	2.13	0.48
1:B:414:LYS:HE3	1:B:488:PHE:O	2.14	0.48
1:B:532:LEU:HD21	1:B:547:VAL:HG11	1.96	0.48
1:A:23:VAL:HG13	1:A:70:PHE:HE2	1.77	0.48
1:B:39:HIS:O	1:B:43:VAL:HG23	2.13	0.48
1:B:152:PRO:HB2	1:B:257:ARG:HH11	1.78	0.48
1:B:367:HIS:O	1:B:371:ALA:HB2	2.13	0.48
1:B:376:GLU:O	1:B:379:PRO:HD2	2.14	0.47
1:B:464:HIS:CG	1:B:473:VAL:HG11	2.48	0.47
1:A:564:LYS:HB3	1:A:567:CYS:HB3	1.96	0.47
1:A:433:VAL:HG23	1:A:452:TYR:HD2	1.78	0.47
1:A:305:LEU:HD13	1:A:334:TYR:CD2	2.50	0.47
1:A:510:HIS:HA	1:A:568:PHE:CB	2.45	0.47
1:A:26:ALA:HB2	1:A:250:LEU:HD12	1.96	0.47
1:A:194:ALA:HB1	1:A:455:VAL:CG1	2.45	0.47
1:A:449:ALA:O	1:A:453:LEU:HG	2.15	0.47
1:B:25:ILE:HD13	1:B:154:LEU:HD23	1.95	0.47
1:B:281:LYS:HD2	1:B:285:GLU:CG	2.43	0.47
1:B:545:LYS:HA	1:B:548:MET:HB2	1.95	0.47
1:B:558:CYS:SG	1:B:571:GLU:HB3	2.55	0.47
1:A:507:PHE:CD1	1:A:507:PHE:N	2.83	0.47
1:B:179:LEU:CB	1:B:180:PRO:HD3	2.42	0.47
1:A:25:ILE:HD13	1:A:154:LEU:HD23	1.96	0.47
1:A:39:HIS:HD2	1:A:140:TYR:CE1	2.32	0.47
1:A:387:LEU:HD11	2:A:2002:C1F:H9C2	1.97	0.46
1:A:410:ARG:NH1	2:A:2002:C1F:C4	2.76	0.46
1:A:553:ALA:HA	1:A:556:GLU:HG2	1.96	0.46
1:A:529:LEU:HD22	1:A:548:MET:CE	2.45	0.46
1:B:408:LEU:HD22	1:B:530:VAL:HG22	1.98	0.46
1:B:420:THR:O	1:B:424:VAL:HG23	2.16	0.46
1:B:57:GLU:O	1:B:58:SER:C	2.54	0.46
1:A:39:HIS:HD2	1:A:140:TYR:HE1	1.62	0.46
1:B:388:ILE:HD12	1:B:449:ALA:CB	2.46	0.46
1:B:516:LEU:N	1:B:516:LEU:CD1	2.67	0.45
1:A:170:GLN:HG3	1:A:170:GLN:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:ARG:HG3	1:B:117:ARG:O	2.17	0.45
1:A:525:LYS:HG2	1:A:551:PHE:CD2	2.52	0.45
1:B:522:GLN:HA	1:B:525:LYS:HD3	1.98	0.45
1:A:554:PHE:N	1:A:554:PHE:CD2	2.83	0.45
1:B:95:GLU:OE1	1:B:99:ASN:CB	2.58	0.45
1:A:529:LEU:HD13	1:A:548:MET:HE1	1.99	0.44
1:B:464:HIS:CE1	1:B:469:VAL:H	2.35	0.44
1:A:49:PHE:C	1:A:49:PHE:CD2	2.90	0.44
1:B:27:PHE:HE1	1:B:70:PHE:CD2	2.35	0.44
1:B:408:LEU:HD22	1:B:530:VAL:CG2	2.48	0.44
1:B:543:GLN:O	1:B:546:ALA:HB3	2.17	0.44
1:A:61:ASN:HD22	1:A:64:LYS:CE	2.28	0.44
1:A:72:ASP:O	1:A:76:THR:HG23	2.18	0.44
1:A:276:LYS:HD3	1:A:277:GLU:H	1.82	0.44
1:B:57:GLU:CG	1:B:58:SER:H	2.16	0.44
1:A:497:TYR:HE2	1:A:537:PRO:HG3	1.83	0.44
1:B:26:ALA:HB2	1:B:250:LEU:HD12	1.99	0.44
1:B:138:TYR:O	1:B:142:ILE:HG12	2.18	0.44
1:B:433:VAL:HG21	1:B:453:LEU:HD21	2.00	0.44
1:B:274:LYS:CE	1:B:296:ASP:HA	2.48	0.44
1:B:381:VAL:O	1:B:384:PRO:HD2	2.17	0.44
1:A:404:GLN:HG2	1:A:431:GLY:HA3	2.00	0.43
1:B:10:ARG:O	1:B:14:LEU:HD23	2.17	0.43
1:A:155:LEU:HD23	1:A:155:LEU:HA	1.82	0.43
1:A:453:LEU:HD11	2:A:2002:C1F:H121	1.99	0.43
1:A:511:ALA:O	1:A:514:CYS:SG	2.76	0.43
1:B:576:VAL:HA	1:B:579:SER:HB2	2.01	0.43
1:A:49:PHE:O	1:A:49:PHE:CD2	2.70	0.43
1:B:30:TYR:CE1	1:B:103:LEU:HD23	2.52	0.43
1:A:174:LYS:O	1:A:175:ALA:C	2.57	0.43
1:B:498:VAL:O	1:B:498:VAL:HG23	2.18	0.43
1:B:225:LYS:HG2	1:B:299:PRO:HG3	2.00	0.42
1:B:370:TYR:CD1	1:B:370:TYR:C	2.92	0.42
1:A:56:ASP:C	1:A:58:SER:H	2.23	0.42
1:A:151:ALA:HB3	1:A:152:PRO:CD	2.42	0.42
1:A:529:LEU:O	1:A:533:VAL:HG23	2.19	0.42
1:B:110:PRO:CB	1:B:112:LEU:HD21	2.48	0.42
1:A:6:GLU:O	1:A:9:HIS:HB3	2.18	0.42
1:A:274:LYS:HA	1:A:276:LYS:HE3	2.01	0.42
1:B:103:LEU:C	1:B:105:HIS:H	2.21	0.42
1:B:408:LEU:HD11	1:B:526:GLN:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:LEU:O	1:A:46:VAL:HG23	2.20	0.42
1:A:529:LEU:HB2	1:A:548:MET:HE1	2.02	0.42
1:A:512:ASP:O	1:A:515:THR:HG22	2.19	0.42
1:B:529:LEU:HD13	1:B:548:MET:HG2	2.01	0.42
1:A:21:ALA:HB1	1:A:155:LEU:HD21	2.02	0.42
1:A:348:ARG:HH22	1:A:450:GLU:CD	2.23	0.42
1:B:252:GLU:OE1	1:B:252:GLU:N	2.36	0.42
1:A:249:ASP:HB3	1:A:252:GLU:CG	2.50	0.42
1:A:356:THR:O	1:A:360:CYS:HB2	2.19	0.42
1:A:66:LEU:O	1:A:70:PHE:CD1	2.71	0.41
1:B:50:ALA:O	1:B:54:VAL:HG23	2.20	0.41
1:B:110:PRO:CB	1:B:112:LEU:CD2	2.87	0.41
1:A:276:LYS:NZ	1:A:277:GLU:HG3	2.35	0.41
1:A:249:ASP:HB3	1:A:252:GLU:CD	2.41	0.41
1:B:560:LYS:O	1:B:560:LYS:HG3	2.20	0.41
1:B:206:PHE:CD2	1:B:481:LEU:HD22	2.55	0.41
1:B:108:ASP:C	1:B:110:PRO:HD3	2.41	0.41
1:A:145:ARG:HG3	1:A:145:ARG:NH1	2.36	0.41
1:B:51:LYS:C	1:B:53:CYS:H	2.24	0.41
1:B:107:ASP:HB3	1:B:110:PRO:HG3	2.02	0.41
1:B:116:VAL:O	1:B:116:VAL:HG13	2.21	0.41
1:B:460:LEU:O	1:B:460:LEU:HD12	2.20	0.41
1:B:513:ILE:O	1:B:513:ILE:HG13	2.21	0.41
1:B:558:CYS:C	1:B:560:LYS:H	2.24	0.41
1:A:408:LEU:CD1	1:A:526:GLN:HB3	2.51	0.41
1:B:260:LEU:O	1:B:264:ILE:HG13	2.21	0.41
1:B:441:PRO:O	1:B:442:GLU:C	2.59	0.41
1:A:281:LYS:HB3	1:A:281:LYS:HE2	1.86	0.40
1:A:555:VAL:O	1:A:559:CYS:HB2	2.20	0.40
1:B:161:TYR:O	1:B:164:ALA:HB3	2.21	0.40
1:B:220:SER:OG	1:B:332:TYR:HD1	2.04	0.40
1:B:529:LEU:O	1:B:533:VAL:HG23	2.21	0.40
1:B:185:LEU:HD23	1:B:185:LEU:HA	1.91	0.40
1:A:333:GLU:OE1	1:A:337:ARG:NH2	2.55	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	565/585 (97%)	514 (91%)	41 (7%)	10 (2%)	8 6
1	B	562/585 (96%)	506 (90%)	43 (8%)	13 (2%)	6 4
All	All	1127/1170 (96%)	1020 (90%)	84 (8%)	23 (2%)	7 5

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	59	ALA
1	A	95	GLU
1	B	54	VAL
1	B	57	GLU
1	B	58	SER
1	B	300	ALA
1	A	58	SER
1	A	300	ALA
1	A	557	LYS
1	A	562	ASP
1	B	442	GLU
1	B	538	LYS
1	B	565	GLU
1	B	283	LEU
1	B	60	GLU
1	B	276	LYS
1	B	281	LYS
1	A	57	GLU
1	A	60	GLU
1	B	118	PRO
1	A	315	VAL
1	B	537	PRO
1	A	77	VAL

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	446/511 (87%)	433 (97%)	13 (3%)	42	52
1	B	431/511 (84%)	418 (97%)	13 (3%)	41	50
All	All	877/1022 (86%)	851 (97%)	26 (3%)	41	50

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	GLU
1	A	49	PHE
1	A	95	GLU
1	A	109	ASN
1	A	252	GLU
1	A	276	LYS
1	A	287	SER
1	A	310	VAL
1	A	435	SER
1	A	442	GLU
1	A	467	THR
1	A	549	ASP
1	A	558	CYS
1	B	38	ASP
1	B	105	HIS
1	B	111	ASN
1	B	112	LEU
1	B	179	LEU
1	B	245	CYS
1	B	304	SER
1	B	344	VAL
1	B	375	ASP
1	B	387	LEU
1	B	513	ILE
1	B	516	LEU
1	B	548	MET

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

Mol	Chain	Res	Type
1	A	29	GLN
1	A	39	HIS
1	A	61	ASN
1	A	109	ASN
1	A	464	HIS
1	A	483	ASN
1	B	9	HIS
1	B	111	ASN
1	B	318	ASN
1	B	338	HIS
1	B	464	HIS
1	B	483	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

4 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	C1F	A	2001	-	11,17,17	1.36	3 (27%)	15,23,23	1.46	3 (20%)
2	C1F	B	2001	-	11,17,17	1.33	2 (18%)	15,23,23	1.42	3 (20%)
2	C1F	B	2002	-	11,17,17	1.35	2 (18%)	15,23,23	1.41	3 (20%)
2	C1F	A	2002	-	11,17,17	1.37	2 (18%)	15,23,23	1.46	4 (26%)

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	C1F	A	2001	-	-	2/8/12/12	0/1/1/1
2	C1F	B	2001	-	-	2/8/12/12	0/1/1/1
2	C1F	B	2002	-	-	3/8/12/12	0/1/1/1
2	C1F	A	2002	-	-	3/8/12/12	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2002	C1F	C2-C13	2.82	1.57	1.50
2	A	2002	C1F	O2-C13	-2.75	1.22	1.30
2	B	2002	C1F	O2-C13	-2.70	1.22	1.30
2	B	2001	C1F	O2-C13	-2.50	1.22	1.30
2	A	2001	C1F	C2-C13	2.46	1.56	1.50
2	B	2002	C1F	C2-C13	2.43	1.56	1.50
2	B	2001	C1F	C2-C13	2.35	1.56	1.50
2	A	2001	C1F	O2-C13	-2.34	1.23	1.30
2	A	2001	C1F	O4-C70	-2.15	1.23	1.30

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2002	C1F	O2-C13-O1	-2.89	116.92	123.35
2	B	2002	C1F	O2-C13-O1	-2.71	117.33	123.35
2	B	2001	C1F	O2-C13-O1	-2.67	117.43	123.35
2	A	2001	C1F	O2-C13-O1	-2.64	117.50	123.35
2	A	2001	C1F	C6-C1-C2	2.47	129.29	124.68
2	A	2002	C1F	O2-C13-C2	2.45	121.85	114.75
2	A	2001	C1F	O2-C13-C2	2.45	121.85	114.75
2	B	2001	C1F	O2-C13-C2	2.39	121.67	114.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2002	C1F	O2-C13-C2	2.37	121.62	114.75
2	B	2001	C1F	C6-C1-C2	2.35	129.07	124.68
2	B	2002	C1F	C6-C1-C2	2.33	129.04	124.68
2	A	2002	C1F	C6-C1-C2	2.15	128.71	124.68
2	A	2002	C1F	O4-C70-C9	2.07	120.68	114.03

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2002	C1F	C40-C11-C12-C7
2	B	2002	C1F	C40-C11-C12-C7
2	A	2001	C1F	O3-C70-C9-C4
2	A	2002	C1F	O3-C70-C9-C4
2	A	2001	C1F	O4-C70-C9-C4
2	B	2002	C1F	O4-C70-C9-C4
2	B	2002	C1F	O3-C70-C9-C4
2	A	2002	C1F	O4-C70-C9-C4
2	B	2001	C1F	O4-C70-C9-C4
2	B	2001	C1F	O3-C70-C9-C4

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2001	C1F	1	0
2	B	2001	C1F	1	0
2	B	2002	C1F	1	0
2	A	2002	C1F	4	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	569/585 (97%)	0.08	25 (4%)	34	46	27, 62, 135, 144	0
1	B	566/585 (96%)	0.17	31 (5%)	25	36	25, 66, 132, 150	0
All	All	1135/1170 (97%)	0.13	56 (4%)	29	42	25, 65, 135, 150	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	563	ASP	6.6
1	B	562	ASP	6.4
1	B	508	THR	6.1
1	B	568	PHE	6.0
1	A	555	VAL	5.3
1	B	566	THR	5.2
1	B	507	PHE	5.1
1	B	54	VAL	4.9
1	B	559	CYS	4.9
1	B	577	ALA	4.6
1	A	569	ALA	4.5
1	A	560	LYS	4.5
1	B	564	LYS	4.5
1	B	546	ALA	4.4
1	A	508	THR	4.4
1	B	578	ALA	4.2
1	A	559	CYS	3.8
1	B	558	CYS	3.8
1	B	504	ALA	3.7
1	B	575	LEU	3.7
1	A	561	ALA	3.7
1	B	563	ASP	3.6
1	A	578	ALA	3.4
1	A	504	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	510	HIS	3.3
1	A	577	ALA	3.3
1	B	509	PHE	3.3
1	A	562	ASP	3.2
1	A	59	ALA	3.1
1	B	560	LYS	3.1
1	A	513	ILE	3.1
1	B	551	PHE	3.0
1	A	510	HIS	2.9
1	A	511	ALA	2.9
1	B	503	ASN	2.9
1	B	502	PHE	2.8
1	A	575	LEU	2.7
1	A	551	PHE	2.7
1	B	40	VAL	2.7
1	B	513	ILE	2.7
1	A	503	ASN	2.7
1	A	579	SER	2.5
1	B	55	ALA	2.5
1	B	561	ALA	2.5
1	B	56	ASP	2.4
1	A	554	PHE	2.3
1	A	570	GLU	2.3
1	A	509	PHE	2.3
1	B	570	GLU	2.3
1	A	553	ALA	2.3
1	B	116	VAL	2.2
1	B	580	GLN	2.2
1	B	139	LEU	2.2
1	A	558	CYS	2.1
1	B	505	GLU	2.1
1	A	568	PHE	2.1

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 monosaccharides 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	C1F	B	2002	17/17	0.82	0.31	82,85,95,95	0
2	C1F	A	2002	17/17	0.83	0.30	81,86,96,96	0
2	C1F	B	2001	17/17	0.95	0.16	63,64,67,67	0
2	C1F	A	2001	17/17	0.97	0.14	58,66,72,74	0

6.5 Other polymers (i)

There are no such residues in this entry.