Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 12:51 AM GMT

PDB ID	:	2BXF
Title	:	HUMAN SERUM ALBUMIN COMPLEXED WITH DIAZEPAM
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 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

http://wwpdb.org/validation/2016/XrayValidationReportHelp

with specific help available everywhere you see the (i) symbol.

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865
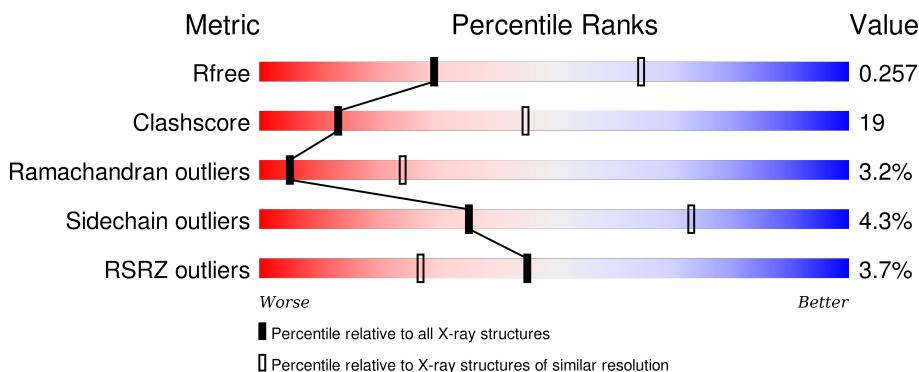
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
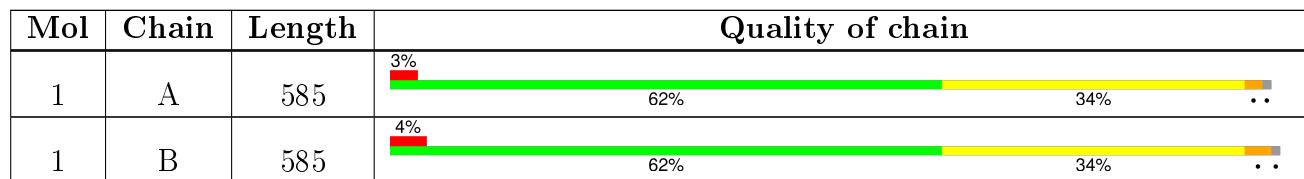
The reported resolution of this entry is 2.95 Å.

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}	91344	2184 (3.00-2.92)
Clashscore	102246	2552 (3.00-2.92)
Ramachandran outliers	100387	2468 (3.00-2.92)
Sidechain outliers	100360	2471 (3.00-2.92)
RSRZ outliers	91569	2201 (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. 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	3% 62% 34% ··
1	B	585	4% 62% 34% ··

2 Entry composition (i)
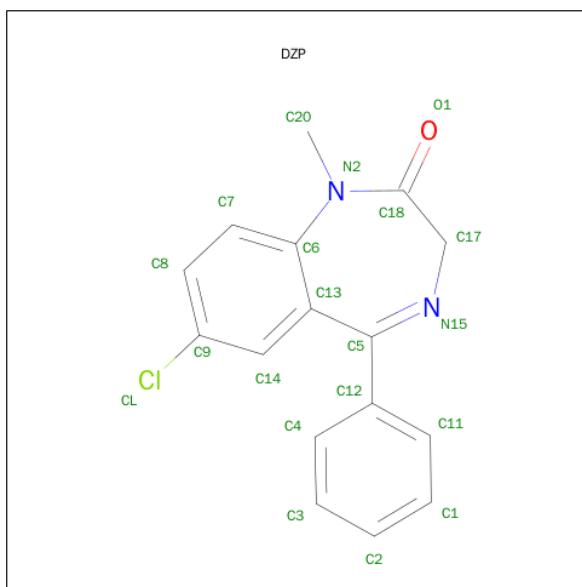
There are 2 unique types of molecules in this entry. The entry contains 8615 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
1	A	578	Total	C	N	O	S	0	0	0
			4282	2700	713	828	41			
1	B	578	Total	C	N	O	S	0	0	0
			4293	2711	714	828	40			

- Molecule 2 is 7-CHLORO-1-METHYL-5-PHENYL-1,3-DIHYDRO-2H-1,4-BENZODIAZEP IN-2-ONE (three-letter code: DZP) (formula: $C_{16}H_{13}ClN_2O$).
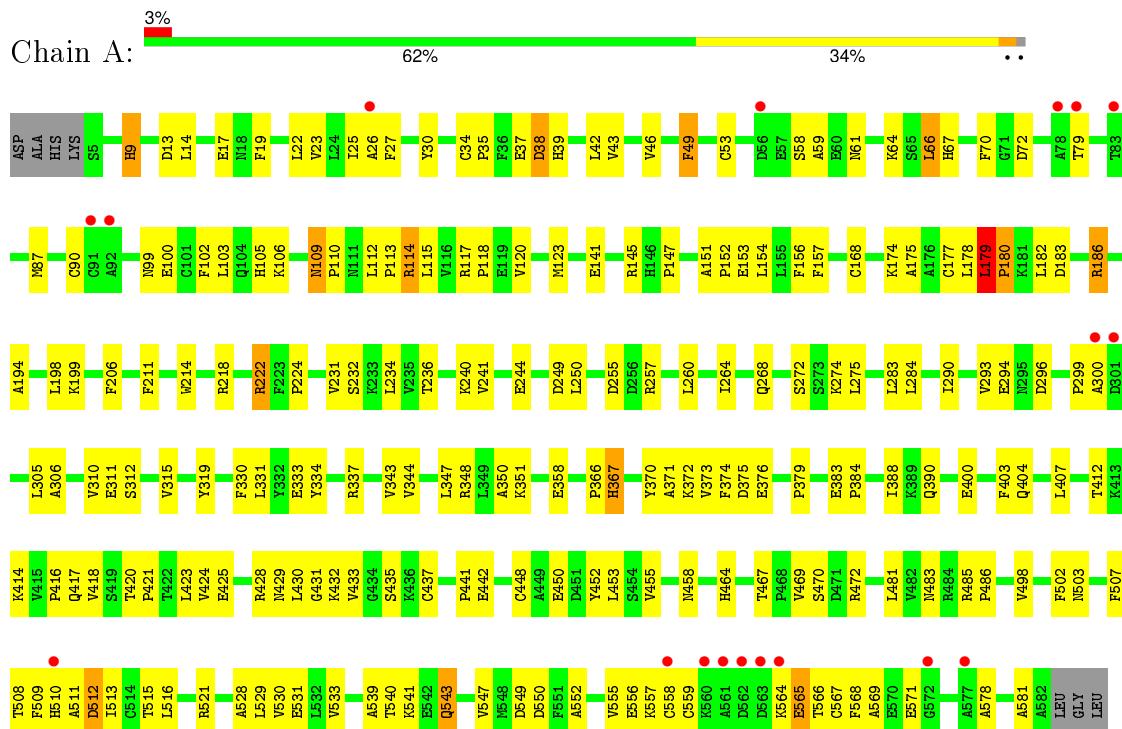
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			20	16	1	2	1		
2	B	1	Total	C	Cl	N	O	0	0
			20	16	1	2	1		
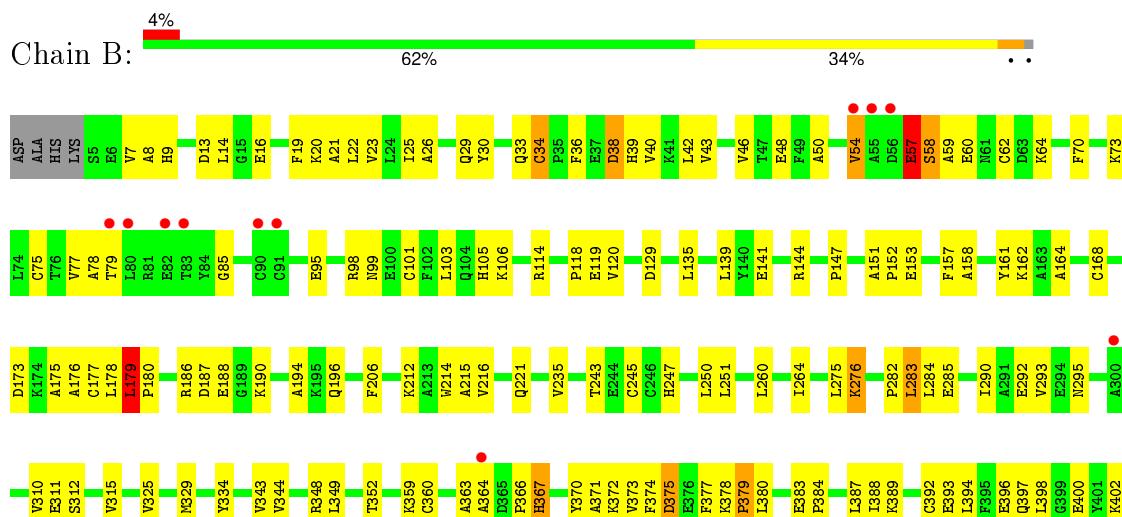
3 Residue-property plots ⓘ
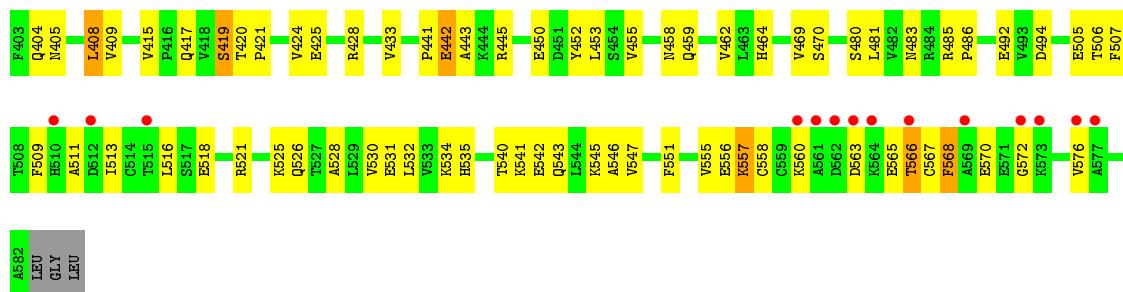
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 1: SERUM ALBUMIN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	55.29Å 55.78Å 120.51Å 81.17° 90.22° 65.93°	Depositor
Resolution (Å)	22.59 – 2.95 22.59 – 2.95	Depositor EDS
% Data completeness (in resolution range)	96.7 (22.59-2.95) 90.9 (22.59-2.95)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.62 (at 2.94Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.215 , 0.262 0.213 , 0.257	Depositor DCC
R_{free} test set	1243 reflections (4.72%)	DCC
Wilson B-factor (Å^2)	71.2	Xtriage
Anisotropy	0.308	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 74.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|> = 0.49$, $<L^2> = 0.33$	Xtriage
Outliers	0 of 27216 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8615	wwPDB-VP
Average B, all atoms (Å^2)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.38% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: DZP

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	0.38	0/4366	0.61	0/5949
1	B	0.38	0/4377	0.60	0/5961
All	All	0.38	0/8743	0.60	0/11910

There are no bond length outliers.

There are no bond angle outliers.

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	4282	0	3874	153	0
1	B	4293	0	3908	156	0
2	A	20	0	13	0	0
2	B	20	0	13	1	0
All	All	8615	0	7808	309	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 19.

All (309) 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:B:540:THR:HG22	1:B:541:LYS:H	1.03	1.08
1:B:383:GLU:HB3	1:B:384:PRO:HD3	1.48	0.94
1:A:540:THR:HG22	1:A:541:LYS:H	1.33	0.94
1:B:424:VAL:O	1:B:428:ARG:HG3	1.67	0.93
1:A:424:VAL:O	1:A:428:ARG:HG3	1.70	0.92
1:B:540:THR:HG22	1:B:541:LYS:N	1.87	0.87
1:B:394:LEU:O	1:B:397:GLN:HG2	1.78	0.83
1:A:214:TRP:CD1	1:A:343:VAL:HG11	2.13	0.82
1:B:540:THR:CG2	1:B:541:LYS:H	1.85	0.82
1:B:433:VAL:HG22	1:B:452:TYR:HD2	1.44	0.82
1:A:151:ALA:HB3	1:A:152:PRO:HD3	1.61	0.82
1:B:419:SER:OG	1:B:421:PRO:HD2	1.81	0.80
1:B:206:PHE:CE2	1:B:481:LEU:HD13	2.19	0.78
1:A:23:VAL:HG13	1:A:70:PHE:HE2	1.49	0.77
1:B:480:SER:OG	1:B:483:ASN:HB2	1.84	0.77
1:B:483:ASN:O	1:B:486:PRO:HD2	1.84	0.76
1:A:152:PRO:HB2	1:A:257:ARG:HH11	1.49	0.76
1:B:151:ALA:HB3	1:B:152:PRO:HD3	1.68	0.76
1:A:224:PRO:HB2	1:A:299:PRO:HD3	1.66	0.75
1:B:135:LEU:HD11	1:B:162:LYS:HD3	1.68	0.75
1:B:16:GLU:O	1:B:20:LYS:HG2	1.86	0.75
1:A:483:ASN:O	1:A:486:PRO:HD2	1.86	0.74
1:B:383:GLU:OE2	1:B:387:LEU:HD11	1.88	0.74
1:A:540:THR:HG22	1:A:541:LYS:N	2.04	0.72
1:A:120:VAL:HG21	1:A:175:ALA:HA	1.72	0.70
1:B:531:GLU:O	1:B:535:HIS:HD2	1.74	0.70
1:A:420:THR:O	1:A:424:VAL:HG23	1.91	0.69
1:B:120:VAL:HG21	1:B:175:ALA:HA	1.74	0.69
1:B:325:VAL:HG12	1:B:329:MET:CE	2.24	0.68
1:B:194:ALA:HB1	1:B:455:VAL:CG1	2.25	0.67
1:A:531:GLU:HA	1:A:531:GLU:OE1	1.93	0.67
1:B:433:VAL:HG22	1:B:452:TYR:CD2	2.28	0.66
1:B:378:LYS:HB2	1:B:379:PRO:HD3	1.77	0.66
1:A:183:ASP:O	1:A:186:ARG:HG2	1.96	0.66
1:B:392:CYS:O	1:B:396:GLU:HG3	1.95	0.66
1:A:61:ASN:HB3	1:A:64:LYS:HD3	1.78	0.65
1:A:168:CYS:SG	1:A:177:CYS:C	2.75	0.65
1:B:30:TYR:HE1	1:B:103:LEU:HD23	1.61	0.65
1:A:464:HIS:HE1	1:A:470:SER:H	1.43	0.65
1:A:152:PRO:CB	1:A:257:ARG:HH11	2.09	0.65
1:B:39:HIS:O	1:B:43:VAL:HG23	1.97	0.64
1:A:512:ASP:O	1:A:515:THR:HG22	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:GLU:O	1:A:379:PRO:HD2	1.97	0.63
1:B:34:CYS:HB3	1:B:39:HIS:NE2	2.14	0.63
1:B:106:LYS:HD3	1:B:147:PRO:HB2	1.79	0.63
1:B:359:LYS:HG3	1:B:360:CYS:N	2.13	0.63
1:B:59:ALA:HB3	1:B:62:CYS:SG	2.39	0.62
1:A:117:ARG:HH12	1:A:182:LEU:HB3	1.63	0.62
1:A:567:CYS:O	1:A:571:GLU:HB2	1.99	0.62
1:B:521:ARG:NH1	1:B:521:ARG:HB2	2.15	0.62
1:B:325:VAL:HG12	1:B:329:MET:HE2	1.81	0.62
1:A:194:ALA:HB1	1:A:455:VAL:CG1	2.30	0.62
1:A:539:ALA:HB1	1:A:543:GLN:HG3	1.81	0.62
1:B:464:HIS:CE1	1:B:469:VAL:H	2.17	0.62
1:B:572:GLY:O	1:B:576:VAL:HG23	2.00	0.61
1:A:540:THR:CG2	1:A:541:LYS:H	2.12	0.61
1:A:152:PRO:HB2	1:A:257:ARG:NH1	2.14	0.61
1:A:206:PHE:CD2	1:A:481:LEU:HD22	2.35	0.61
1:A:117:ARG:NH1	1:A:182:LEU:HB3	2.15	0.61
1:B:516:LEU:O	1:B:521:ARG:NH2	2.27	0.61
1:A:433:VAL:HG22	1:A:452:TYR:CD2	2.35	0.61
1:A:483:ASN:C	1:A:486:PRO:HD2	2.21	0.61
1:A:367:HIS:O	1:A:371:ALA:HB2	2.01	0.61
1:B:556:GLU:O	1:B:560:LYS:HG2	2.01	0.60
1:B:310:VAL:O	1:B:370:TYR:HE1	1.84	0.60
1:A:556:GLU:HG3	1:A:557:LYS:H	1.65	0.60
1:A:383:GLU:HB3	1:A:384:PRO:CD	2.31	0.60
1:B:372:LYS:O	1:B:375:ASP:HB2	2.00	0.60
1:B:57:GLU:OE1	1:B:57:GLU:HA	2.01	0.59
1:B:98:ARG:O	1:B:101:CYS:HB3	2.02	0.59
1:A:199:LYS:HG2	1:A:211:PHE:HE1	1.67	0.59
1:A:179:LEU:HB2	1:A:180:PRO:HD3	1.84	0.59
1:B:383:GLU:HB3	1:B:384:PRO:CD	2.26	0.59
1:B:485:ARG:HB3	1:B:486:PRO:HD3	1.84	0.59
1:B:511:ALA:HA	1:B:568:PHE:CE2	2.38	0.59
1:A:412:THR:O	1:A:416:PRO:HG3	2.02	0.59
1:A:305:LEU:HD21	1:A:333:GLU:HB3	1.84	0.59
1:A:240:LYS:O	1:A:244:GLU:HG3	2.03	0.59
1:A:87:MET:HE1	1:A:105:HIS:HB3	1.83	0.59
1:B:364:ALA:O	1:B:366:PRO:HD3	2.03	0.58
1:A:507:PHE:O	1:A:507:PHE:CD1	2.56	0.58
1:B:442:GLU:HA	1:B:445:ARG:HD2	1.85	0.58
1:B:120:VAL:HG21	1:B:175:ALA:CA	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:551:PHE:O	1:B:555:VAL:HG23	2.04	0.58
1:B:120:VAL:HG21	1:B:175:ALA:CB	2.34	0.58
1:B:214:TRP:CD1	1:B:343:VAL:HG11	2.39	0.57
1:A:417:GLN:CD	1:A:417:GLN:H	2.07	0.57
1:B:179:LEU:HB2	1:B:180:PRO:HD3	1.87	0.57
1:A:66:LEU:O	1:A:70:PHE:HD1	1.87	0.57
1:B:556:GLU:HG3	1:B:557:LYS:H	1.70	0.57
1:A:214:TRP:NE1	1:A:343:VAL:HG11	2.18	0.57
1:A:400:GLU:O	1:A:404:GLN:HG3	2.05	0.57
1:B:464:HIS:CE1	1:B:470:SER:H	2.23	0.56
1:B:212:LYS:O	1:B:216:VAL:HG23	2.05	0.56
1:B:464:HIS:HE1	1:B:470:SER:H	1.52	0.56
1:A:42:LEU:O	1:A:46:VAL:HG23	2.05	0.56
1:A:110:PRO:HB2	1:A:112:LEU:HG	1.88	0.56
1:B:531:GLU:HA	1:B:531:GLU:OE1	2.05	0.55
1:A:206:PHE:CE2	1:A:481:LEU:HD13	2.41	0.55
1:B:367:HIS:O	1:B:371:ALA:HB2	2.06	0.55
1:B:48:GLU:O	1:B:48:GLU:HG2	2.06	0.55
1:A:529:LEU:O	1:A:533:VAL:HG23	2.07	0.55
1:A:384:PRO:O	1:A:388:ILE:HG12	2.06	0.55
1:B:206:PHE:CD2	1:B:481:LEU:HD22	2.42	0.55
1:B:348:ARG:NH2	1:B:450:GLU:OE2	2.25	0.55
1:B:42:LEU:O	1:B:46:VAL:HG23	2.07	0.55
1:A:433:VAL:HG22	1:A:452:TYR:HD2	1.72	0.54
1:A:556:GLU:HG3	1:A:557:LYS:N	2.22	0.54
1:A:224:PRO:HD2	1:A:296:ASP:HB3	1.89	0.54
1:A:425:GLU:OE1	1:A:425:GLU:HA	2.07	0.54
1:A:578:ALA:O	1:A:581:ALA:HB3	2.07	0.54
1:A:106:LYS:HD3	1:A:147:PRO:HB2	1.90	0.54
1:B:344:VAL:O	1:B:348:ARG:HB2	2.09	0.53
1:A:19:PHE:O	1:A:23:VAL:HG23	2.08	0.53
1:B:542:GLU:O	1:B:545:LYS:HG2	2.10	0.53
1:B:373:VAL:HG13	1:B:374:PHE:HD1	1.74	0.52
1:B:543:GLN:O	1:B:546:ALA:HB3	2.09	0.52
1:B:50:ALA:O	1:B:54:VAL:HG23	2.09	0.52
1:B:75:CYS:HA	1:B:78:ALA:HB3	1.90	0.52
1:B:33:GLN:HE21	1:B:33:GLN:HA	1.73	0.52
1:B:483:ASN:C	1:B:486:PRO:HD2	2.30	0.52
1:A:49:PHE:O	1:A:49:PHE:HD2	1.93	0.52
1:A:543:GLN:O	1:A:547:VAL:HG23	2.10	0.52
1:B:404:GLN:NE2	1:B:428:ARG:HA	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:LEU:HB3	1:A:70:PHE:CE1	2.45	0.51
1:B:511:ALA:C	1:B:513:ILE:H	2.13	0.51
1:B:507:PHE:CD1	1:B:507:PHE:O	2.64	0.51
1:B:186:ARG:O	1:B:190:LYS:HG3	2.11	0.51
1:A:306:ALA:HA	1:A:310:VAL:HG22	1.93	0.51
1:B:153:GLU:O	1:B:157:PHE:HD1	1.93	0.51
1:B:389:LYS:O	1:B:393:GLU:HG3	2.11	0.51
1:B:196:GLN:HA	1:B:196:GLN:NE2	2.26	0.51
1:A:414:LYS:O	1:A:472:ARG:NH1	2.44	0.51
1:B:33:GLN:NE2	1:B:33:GLN:HA	2.26	0.50
1:A:509:PHE:O	1:A:568:PHE:CD1	2.64	0.50
1:A:571:GLU:N	1:A:571:GLU:OE1	2.43	0.50
1:A:38:ASP:OD1	1:A:38:ASP:N	2.44	0.50
1:B:505:GLU:O	1:B:506:THR:C	2.50	0.50
1:B:566:THR:O	1:B:570:GLU:N	2.40	0.50
1:B:405:ASN:O	1:B:409:VAL:HG23	2.11	0.50
1:B:344:VAL:HG21	1:B:450:GLU:HG2	1.93	0.50
1:B:492:GLU:OE1	1:B:492:GLU:HA	2.11	0.50
1:B:398:LEU:HB3	1:B:402:LYS:HB2	1.94	0.50
1:A:274:LYS:HD2	1:A:294:GLU:HG3	1.93	0.49
1:A:319:TYR:OH	1:A:358:GLU:HG2	2.12	0.49
1:A:310:VAL:HG23	1:A:311:GLU:N	2.27	0.49
1:B:36:PHE:O	1:B:40:VAL:HG23	2.12	0.49
1:A:420:THR:HB	1:A:421:PRO:HD3	1.94	0.49
1:B:417:GLN:H	1:B:417:GLN:CD	2.16	0.49
1:A:564:LYS:O	1:A:566:THR:N	2.45	0.49
1:A:87:MET:O	1:A:90:CYS:HB2	2.11	0.49
1:A:206:PHE:CE2	1:A:481:LEU:HB2	2.48	0.49
1:A:372:LYS:O	1:A:375:ASP:HB2	2.13	0.49
1:A:502:PHE:HE1	1:A:507:PHE:CE2	2.31	0.49
1:B:214:TRP:NE1	1:B:343:VAL:HG11	2.28	0.49
1:B:168:CYS:SG	1:B:177:CYS:C	2.91	0.48
1:B:556:GLU:HG3	1:B:557:LYS:N	2.28	0.48
1:B:120:VAL:HG21	1:B:175:ALA:HB2	1.95	0.48
1:A:566:THR:C	1:A:568:PHE:N	2.64	0.48
1:B:46:VAL:HG22	1:B:73:LYS:HE3	1.95	0.48
1:B:30:TYR:CE1	1:B:103:LEU:HD23	2.45	0.48
1:B:260:LEU:O	1:B:264:ILE:HG13	2.13	0.48
1:B:531:GLU:O	1:B:535:HIS:CD2	2.62	0.48
1:A:206:PHE:CD2	1:A:481:LEU:HB2	2.49	0.48
1:B:509:PHE:HB3	1:B:568:PHE:CD1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:531:GLU:OE1	1:A:531:GLU:CA	2.59	0.48
1:B:458:ASN:O	1:B:462:VAL:HG22	2.13	0.48
1:B:425:GLU:OE1	1:B:425:GLU:HA	2.14	0.48
1:B:507:PHE:HZ	1:B:576:VAL:HG22	1.79	0.48
1:A:502:PHE:CG	1:A:503:ASN:N	2.81	0.47
1:B:25:ILE:O	1:B:29:GLN:HG3	2.14	0.47
1:B:283:LEU:HD12	1:B:283:LEU:C	2.34	0.47
1:A:115:LEU:HD22	1:A:145:ARG:NH1	2.29	0.47
1:B:400:GLU:O	1:B:404:GLN:HG3	2.13	0.47
1:B:26:ALA:HB2	1:B:250:LEU:HD12	1.96	0.47
1:A:153:GLU:O	1:A:157:PHE:HD1	1.97	0.47
1:A:373:VAL:HG13	1:A:374:PHE:HD1	1.79	0.47
1:B:9:HIS:O	1:B:13:ASP:HB2	2.14	0.47
1:B:19:PHE:O	1:B:23:VAL:HG23	2.14	0.47
1:B:206:PHE:HE2	1:B:481:LEU:HD13	1.77	0.47
1:B:383:GLU:OE2	1:B:387:LEU:CD1	2.61	0.47
1:A:117:ARG:HA	1:A:118:PRO:HD3	1.83	0.47
1:B:558:CYS:SG	1:B:568:PHE:N	2.88	0.47
1:B:178:LEU:O	1:B:179:LEU:C	2.53	0.47
1:B:282:PRO:HB2	1:B:285:GLU:OE1	2.14	0.47
1:A:66:LEU:HB3	1:A:70:PHE:CD1	2.50	0.46
1:A:417:GLN:OE1	1:A:417:GLN:N	2.28	0.46
1:B:33:GLN:CA	1:B:33:GLN:HE21	2.28	0.46
1:A:485:ARG:HB3	1:A:486:PRO:HD3	1.95	0.46
1:A:49:PHE:CD2	1:A:49:PHE:C	2.88	0.46
1:A:502:PHE:CE1	1:A:507:PHE:CE2	3.03	0.46
1:B:70:PHE:HD1	1:B:70:PHE:H	1.63	0.46
1:A:99:ASN:O	1:A:102:PHE:N	2.48	0.46
1:A:198:LEU:HA	1:A:458:ASN:ND2	2.31	0.46
1:B:290:ILE:O	1:B:293:VAL:HG12	2.15	0.46
1:A:566:THR:O	1:A:569:ALA:N	2.49	0.45
1:B:70:PHE:CD1	1:B:70:PHE:N	2.84	0.45
1:A:260:LEU:O	1:A:264:ILE:HG13	2.15	0.45
1:A:283:LEU:HG	1:A:284:LEU:HD23	1.98	0.45
1:B:38:ASP:O	1:B:42:LEU:HG	2.16	0.45
1:A:23:VAL:HG13	1:A:70:PHE:CE2	2.40	0.45
1:B:161:TYR:O	1:B:164:ALA:HB3	2.17	0.45
1:B:243:THR:HG22	1:B:247:HIS:HD2	1.82	0.45
1:B:420:THR:O	1:B:424:VAL:HG23	2.17	0.45
1:B:528:ALA:O	1:B:531:GLU:HB2	2.16	0.45
1:A:418:VAL:HB	1:A:423:LEU:HD21	2.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:GLU:O	1:B:144:ARG:HG2	2.17	0.45
1:B:119:GLU:OE1	1:B:119:GLU:HA	2.17	0.44
1:A:516:LEU:O	1:A:521:ARG:NH2	2.50	0.44
1:A:151:ALA:CB	1:A:152:PRO:HD3	2.42	0.44
1:A:370:TYR:CD1	1:A:370:TYR:C	2.91	0.44
1:A:49:PHE:CE2	1:A:53:CYS:SG	3.11	0.44
1:A:429:ASN:O	1:A:432:LYS:N	2.49	0.44
1:B:14:LEU:CD1	1:B:251:LEU:HD22	2.47	0.44
1:B:530:VAL:HG12	1:B:534:LYS:HD2	2.00	0.44
1:A:344:VAL:HG21	1:A:450:GLU:HG2	2.00	0.44
1:A:528:ALA:O	1:A:531:GLU:HB2	2.17	0.44
1:B:70:PHE:HD1	1:B:70:PHE:N	2.15	0.44
1:B:525:LYS:O	1:B:528:ALA:HB3	2.17	0.44
1:B:139:LEU:HD21	1:B:158:ALA:HB2	1.99	0.44
1:B:173:ASP:OD2	1:B:176:ALA:HB2	2.18	0.44
1:A:509:PHE:O	1:A:510:HIS:C	2.56	0.44
1:B:283:LEU:HG	1:B:284:LEU:HD23	2.00	0.44
1:A:120:VAL:HG11	1:A:174:LYS:CB	2.48	0.43
1:A:511:ALA:C	1:A:513:ILE:H	2.22	0.43
1:B:563:ASP:OD1	1:B:567:CYS:SG	2.76	0.43
1:B:408:LEU:HD12	1:B:526:GLN:HG2	2.01	0.43
1:A:34:CYS:HA	1:A:35:PRO:HD3	1.86	0.43
1:B:359:LYS:CG	1:B:360:CYS:N	2.80	0.43
1:B:221:GLN:O	1:B:295:ASN:HB3	2.18	0.43
1:B:384:PRO:O	1:B:388:ILE:HG12	2.18	0.43
1:B:7:VAL:HG13	1:B:8:ALA:N	2.34	0.43
1:A:30:TYR:HE1	1:A:103:LEU:HD23	1.83	0.43
1:B:215:ALA:HB3	1:B:235:VAL:HG13	2.00	0.43
1:A:168:CYS:SG	1:A:177:CYS:O	2.76	0.43
1:A:333:GLU:OE1	1:A:337:ARG:NH2	2.50	0.43
1:A:290:ILE:O	1:A:293:VAL:HG12	2.19	0.43
1:A:549:ASP:O	1:A:552:ALA:HB3	2.18	0.43
1:A:272:SER:HB3	1:A:275:LEU:HG	2.00	0.43
1:B:367:HIS:HA	1:B:370:TYR:CZ	2.53	0.43
1:A:564:LYS:O	1:A:565:GLU:C	2.57	0.43
1:A:231:VAL:O	1:A:234:LEU:N	2.51	0.43
1:A:420:THR:HG23	1:A:530:VAL:HG11	2.01	0.43
1:A:453:LEU:HD23	1:A:485:ARG:HG3	2.01	0.43
1:A:67:HIS:CE1	1:A:99:ASN:ND2	2.87	0.43
1:B:349:LEU:HD22	1:B:377:PHE:CG	2.54	0.43
1:A:23:VAL:O	1:A:27:PHE:HD1	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:VAL:HG21	1:A:175:ALA:CA	2.45	0.42
1:A:178:LEU:O	1:A:179:LEU:C	2.57	0.42
1:A:441:PRO:O	1:A:442:GLU:C	2.57	0.42
1:A:153:GLU:O	1:A:156:PHE:HB3	2.19	0.42
1:A:331:LEU:HD21	1:A:347:LEU:HD23	2.00	0.42
1:A:151:ALA:HB3	1:A:152:PRO:CD	2.42	0.42
1:A:558:CYS:SG	1:A:568:PHE:CD2	3.12	0.42
1:A:498:VAL:HG13	1:A:498:VAL:O	2.19	0.42
1:A:14:LEU:HD13	1:A:22:LEU:HD12	2.00	0.42
1:B:441:PRO:O	1:B:443:ALA:N	2.52	0.42
1:B:404:GLN:HE21	1:B:428:ARG:HA	1.83	0.42
1:A:113:PRO:O	1:A:114:ARG:C	2.56	0.42
1:A:109:ASN:HD22	1:A:109:ASN:HA	1.54	0.42
1:B:95:GLU:OE1	1:B:99:ASN:HB2	2.19	0.42
1:A:224:PRO:CB	1:A:299:PRO:HD3	2.43	0.42
1:A:464:HIS:CE1	1:A:469:VAL:H	2.38	0.42
1:A:567:CYS:O	1:A:571:GLU:N	2.52	0.42
1:A:344:VAL:O	1:A:348:ARG:HB2	2.20	0.42
1:A:99:ASN:O	1:A:100:GLU:C	2.58	0.42
1:A:429:ASN:O	1:A:431:GLY:N	2.53	0.42
1:A:117:ARG:HB2	1:A:123:MET:CE	2.50	0.42
1:B:187:ASP:O	1:B:188:GLU:C	2.58	0.42
1:A:310:VAL:O	1:A:370:TYR:HE1	2.03	0.42
1:B:420:THR:HG23	1:B:530:VAL:HG11	2.02	0.41
1:B:275:LEU:O	1:B:276:LYS:C	2.58	0.41
1:A:511:ALA:O	1:A:513:ILE:N	2.53	0.41
1:A:558:CYS:SG	1:A:568:PHE:N	2.93	0.41
1:A:555:VAL:O	1:A:559:CYS:HB2	2.19	0.41
1:A:39:HIS:O	1:A:43:VAL:HG23	2.20	0.41
1:A:437:CYS:SG	1:A:448:CYS:C	2.98	0.41
1:B:532:LEU:HD11	1:B:547:VAL:HG11	2.02	0.41
1:B:518:GLU:O	1:B:521:ARG:HB3	2.20	0.41
1:B:370:TYR:C	1:B:370:TYR:CD1	2.93	0.41
1:B:532:LEU:HA	1:B:532:LEU:HD23	1.96	0.41
1:A:403:PHE:CE2	1:A:407:LEU:HD11	2.55	0.41
1:B:521:ARG:HB2	1:B:521:ARG:HH11	1.85	0.41
1:B:311:GLU:O	1:B:312:SER:C	2.58	0.41
1:A:26:ALA:HB2	1:A:250:LEU:HD12	2.01	0.41
1:B:179:LEU:CB	1:B:180:PRO:HD3	2.51	0.41
1:A:25:ILE:HD13	1:A:154:LEU:HD23	2.03	0.41
1:B:168:CYS:SG	1:B:178:LEU:N	2.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:ASP:O	1:B:190:LYS:N	2.53	0.41
1:B:310:VAL:HG21	1:B:374:PHE:CE1	2.56	0.41
1:A:179:LEU:H	1:A:179:LEU:HD23	1.84	0.41
1:B:48:GLU:O	1:B:48:GLU:CG	2.69	0.41
1:A:9:HIS:ND1	1:A:13:ASP:OD2	2.53	0.41
1:B:57:GLU:O	1:B:59:ALA:N	2.54	0.40
1:A:49:PHE:HD2	1:A:49:PHE:C	2.25	0.40
1:A:232:SER:O	1:A:236:THR:OG1	2.36	0.40
1:B:453:LEU:HD13	2:B:2001:DZP:H203	2.02	0.40
1:A:508:THR:CG2	1:A:509:PHE:N	2.84	0.40
1:B:141:GLU:OE1	1:B:144:ARG:HD3	2.21	0.40
1:B:14:LEU:HD13	1:B:22:LEU:HD12	2.04	0.40
1:A:507:PHE:C	1:A:507:PHE:CD1	2.95	0.40
1:A:511:ALA:HA	1:A:568:PHE:CE2	2.56	0.40
1:B:57:GLU:HB3	1:B:58:SER:H	1.47	0.40
1:A:141:GLU:OE1	1:A:141:GLU:HA	2.22	0.40
1:A:330:PHE:HE2	1:A:350:ALA:HA	1.86	0.40
1:A:218:ARG:HH21	1:A:222:ARG:HH21	1.70	0.40
1:B:21:ALA:O	1:B:25:ILE:HG13	2.22	0.40
1:B:494:ASP:OD1	1:B:494:ASP:C	2.59	0.40
1:A:351:LYS:HA	1:A:351:LYS:HD2	1.87	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	576/585 (98%)	481 (84%)	78 (14%)	17 (3%)	5	26
1	B	576/585 (98%)	490 (85%)	66 (12%)	20 (4%)	4	22
All	All	1152/1170 (98%)	971 (84%)	144 (12%)	37 (3%)	5	24

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	59	ALA
1	A	300	ALA
1	A	565	GLU
1	B	54	VAL
1	B	57	GLU
1	B	58	SER
1	B	60	GLU
1	B	129	ASP
1	A	17	GLU
1	A	58	SER
1	B	85	GLY
1	B	114	ARG
1	B	276	LYS
1	B	565	GLU
1	A	312	SER
1	A	367	HIS
1	A	512	ASP
1	B	363	ALA
1	B	367	HIS
1	B	442	GLU
1	A	430	LEU
1	B	64	LYS
1	B	557	LYS
1	A	114	ARG
1	A	179	LEU
1	A	180	PRO
1	A	255	ASP
1	B	77	VAL
1	B	379	PRO
1	B	380	LEU
1	A	366	PRO
1	A	390	GLN
1	B	118	PRO
1	A	241	VAL
1	A	315	VAL
1	B	179	LEU
1	B	315	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	421/511 (82%)	403 (96%)	18 (4%)	35	73
1	B	424/511 (83%)	406 (96%)	18 (4%)	36	74
All	All	845/1022 (83%)	809 (96%)	36 (4%)	35	73

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	HIS
1	A	37	GLU
1	A	38	ASP
1	A	49	PHE
1	A	66	LEU
1	A	72	ASP
1	A	79	THR
1	A	109	ASN
1	A	179	LEU
1	A	186	ARG
1	A	222	ARG
1	A	249	ASP
1	A	268	GLN
1	A	334	TYR
1	A	435	SER
1	A	467	THR
1	A	543	GLN
1	A	550	ASP
1	B	34	CYS
1	B	38	ASP
1	B	57	GLU
1	B	79	THR
1	B	105	HIS
1	B	179	LEU
1	B	245	CYS
1	B	283	LEU
1	B	292	GLU

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Mol	Chain	Res	Type
1	B	334	TYR
1	B	352	THR
1	B	375	ASP
1	B	408	LEU
1	B	415	VAL
1	B	419	SER
1	B	459	GLN
1	B	566	THR
1	B	568	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	ASN
1	A	196	GLN
1	A	338	HIS
1	A	367	HIS
1	A	464	HIS
1	A	483	ASN
1	B	33	GLN
1	B	99	ASN
1	B	196	GLN
1	B	247	HIS
1	B	385	GLN
1	B	404	GLN
1	B	464	HIS
1	B	483	ASN
1	B	535	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)

2 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	DZP	A	2001	-	22,22,22	1.61	6 (27%)	30,31,31	0.75	0
2	DZP	B	2001	-	22,22,22	1.58	4 (18%)	30,31,31	0.78	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	DZP	A	2001	-	-	0/4/21/21	0/3/3/3
2	DZP	B	2001	-	-	0/4/21/21	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2001	DZP	C8-C7	2.09	1.42	1.38
2	B	2001	DZP	C13-C6	2.16	1.44	1.41
2	A	2001	DZP	C5-N15	2.16	1.31	1.28
2	A	2001	DZP	C12-C5	2.22	1.52	1.49
2	A	2001	DZP	C13-C6	2.45	1.45	1.41
2	A	2001	DZP	C11-C12	2.46	1.43	1.39
2	B	2001	DZP	C18-N2	2.49	1.41	1.37
2	B	2001	DZP	C5-N15	2.61	1.32	1.28
2	A	2001	DZP	C4-C12	2.63	1.43	1.39
2	B	2001	DZP	C4-C12	2.91	1.44	1.39

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2001	DZP	1	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	578/585 (98%)	-0.23	18 (3%)	52	33	33, 77, 141, 154	0
1	B	578/585 (98%)	-0.19	25 (4%)	39	23	35, 80, 145, 159	0
All	All	1156/1170 (98%)	-0.21	43 (3%)	45	27	33, 78, 144, 159	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	55	ALA	5.0
1	B	576	VAL	4.8
1	B	90	CYS	4.5
1	A	79	THR	4.4
1	B	91	CYS	4.3
1	B	569	ALA	4.2
1	B	564	LYS	3.9
1	A	572	GLY	3.8
1	B	562	ASP	3.3
1	B	572	GLY	3.3
1	B	515	THR	3.1
1	A	78	ALA	3.0
1	A	561	ALA	3.0
1	A	562	ASP	3.0
1	A	301	ASP	3.0
1	B	300	ALA	2.9
1	B	83	THR	2.9
1	A	558	CYS	2.9
1	A	91	CYS	2.9
1	B	566	THR	2.6
1	A	564	LYS	2.6
1	B	510	HIS	2.6
1	A	56	ASP	2.6
1	B	56	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	79	THR	2.5
1	B	573	LYS	2.5
1	A	510	HIS	2.4
1	A	563	ASP	2.4
1	B	560	LYS	2.4
1	B	82	GLU	2.3
1	B	512	ASP	2.3
1	A	560	LYS	2.3
1	B	577	ALA	2.3
1	B	364	ALA	2.2
1	B	54	VAL	2.2
1	A	83	THR	2.2
1	B	563	ASP	2.1
1	A	577	ALA	2.1
1	A	300	ALA	2.1
1	A	26	ALA	2.1
1	A	92	ALA	2.1
1	B	561	ALA	2.1
1	B	80	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no 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. 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	RSCC	RSR	LLDF	B-factors($Å^2$)	Q<0.9
2	DZP	A	2001	20/20	0.96	0.23	1.51	50,56,60,62	0
2	DZP	B	2001	20/20	0.96	0.23	1.50	57,58,63,63	0

6.5 Other polymers (i)

There are no such residues in this entry.