



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:39 PM GMT

PDB ID : 1ULV
Title : Crystal Structure of Glucodextranase Complexed with Acarbose
Authors : Mizuno, M.; Tonozuka, T.; Suzuki, S.; Uotsu-Tomita, R.; Kamitori, S.;
Nishikawa, A.; Sakano, Y.
Deposited on : 2003-09-16
Resolution : 2.42 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

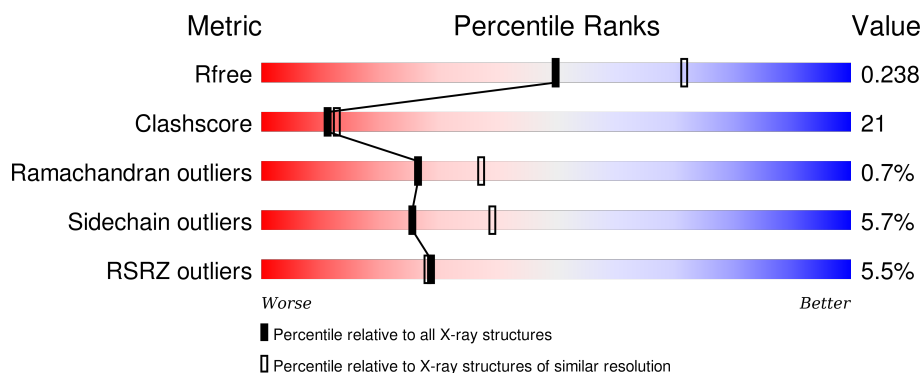
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.42 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	3386 (2.44-2.40)
Clashscore	102246	3897 (2.44-2.40)
Ramachandran outliers	100387	3837 (2.44-2.40)
Sidechain outliers	100360	3838 (2.44-2.40)
RSRZ outliers	91569	3396 (2.44-2.40)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1020	<div> <div>5%</div> <div>67%</div> <div>30%</div> <div>.</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ACR	A	3000	-	-	-	X

2 Entry composition [i](#)

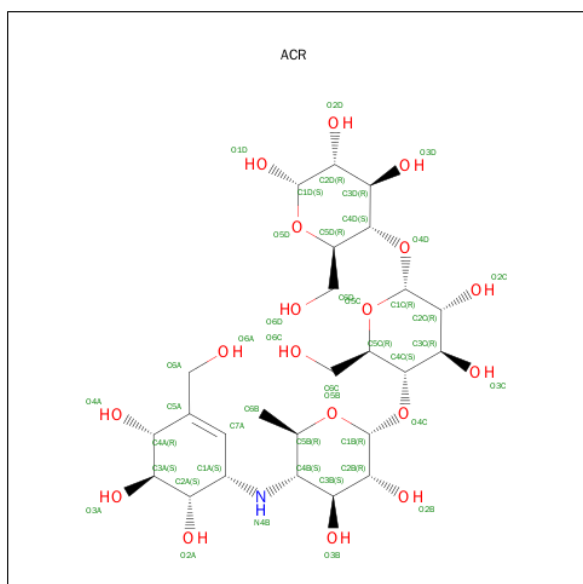
There are 4 unique types of molecules in this entry. The entry contains 7980 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 glucodextranase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1019	Total	C	N	O	S	0	0	0
			7506	4681	1286	1527	12			

- Molecule 2 is SUGAR (ACARBOSE) (three-letter code: ACR) (formula: C₂₅H₄₃NO₁₈).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			32	19	1	12		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	6	Total	Ca	0	0
			6	6		

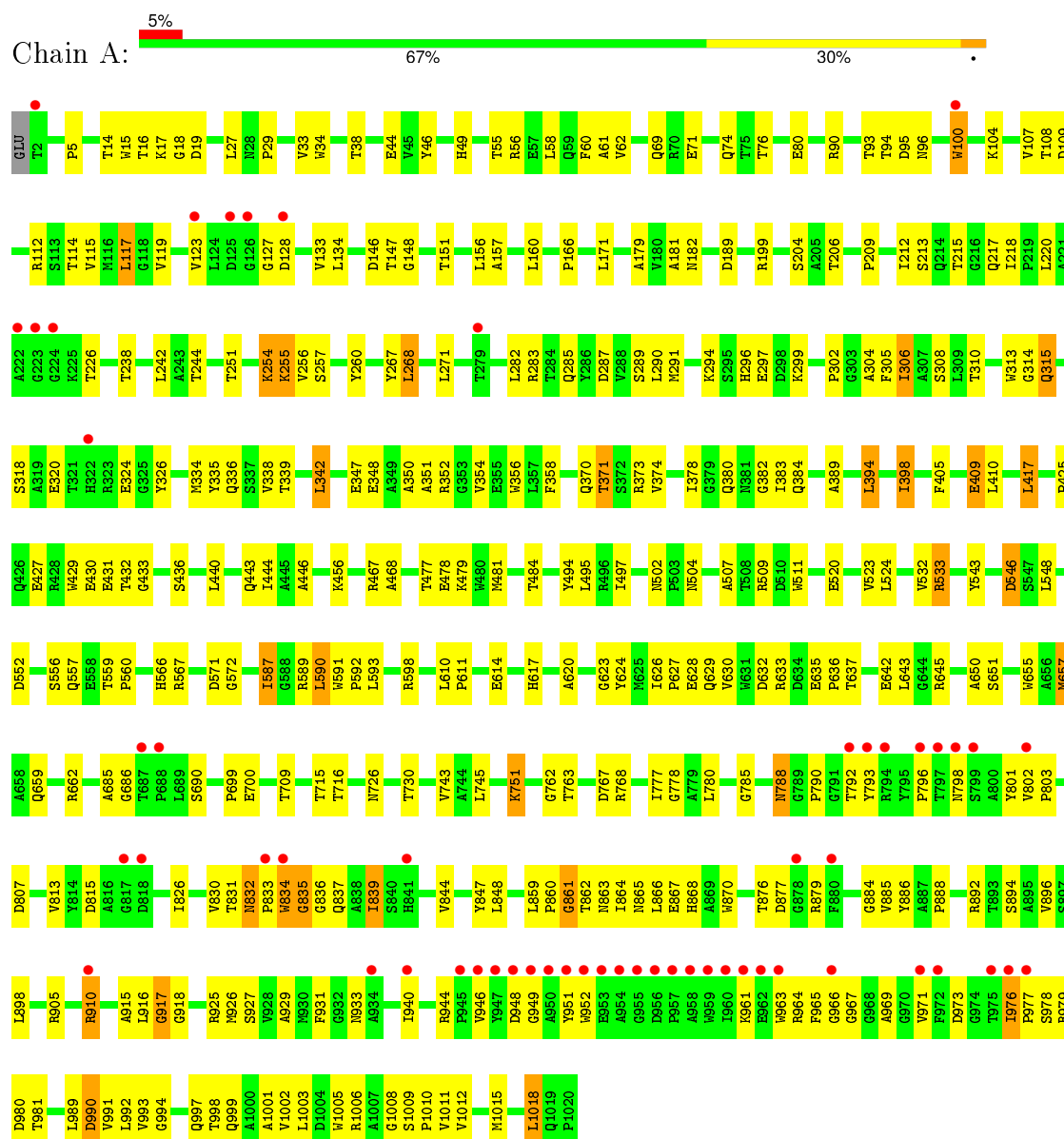
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	436	Total 436	O 436	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: glucodextranase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	198.79Å 88.25Å 80.99Å 90.00° 112.55° 90.00°	Depositor
Resolution (Å)	49.59 – 2.42 49.59 – 2.42	Depositor EDS
% Data completeness (in resolution range)	98.0 (49.59-2.42) 98.1 (49.59-2.42)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.27 (at 2.42Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.196 , 0.238 0.196 , 0.238	Depositor DCC
R_{free} test set	4918 reflections (10.10%)	DCC
Wilson B-factor (Å ²)	20.1	Xtriage
Anisotropy	0.496	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 49.3	EDS
Estimated twinning fraction	0.021 for -h-2*k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 48692 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7980	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: ACR, CA

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	0.33	0/7683	0.61	1/10508 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	546	ASP	CB-CG-OD1	7.20	124.78	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7506	0	7137	305	0
2	A	32	0	31	2	0
3	A	6	0	0	0	0
4	A	436	0	0	14	0
All	All	7980	0	7168	305	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 21.

All (305) 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:133:VAL:HG23	1:A:218:ILE:HD11	1.28	1.14
1:A:371:THR:HG22	1:A:380:GLN:H	1.12	1.14
1:A:29:PRO:HA	1:A:299:LYS:HD2	1.37	1.06
1:A:313:TRP:HA	1:A:315:GLN:HE22	1.23	1.02
1:A:831:THR:HG22	1:A:833:PRO:HD3	1.44	1.00
1:A:104:LYS:HB3	1:A:117:LEU:HD21	1.41	0.99
1:A:123:VAL:HG11	1:A:127:GLY:HA2	1.43	0.96
1:A:285:GLN:HE21	1:A:617:HIS:HD2	1.03	0.96
1:A:339:THR:HG21	1:A:662:ARG:HH21	1.35	0.91
1:A:358:PHE:HB3	1:A:409:GLU:HG3	1.53	0.90
1:A:285:GLN:HE21	1:A:617:HIS:CD2	1.94	0.84
1:A:342:LEU:HD11	1:A:398:ILE:HD11	1.59	0.84
1:A:133:VAL:CG2	1:A:218:ILE:HD11	2.08	0.83
1:A:370:GLN:HE21	1:A:382:GLY:H	1.24	0.83
1:A:342:LEU:HD21	1:A:398:ILE:HD13	1.62	0.82
1:A:925:ARG:HB3	1:A:1015:MET:HG3	1.61	0.80
1:A:17:LYS:HD3	1:A:19:ASP:HB3	1.63	0.80
1:A:339:THR:HG23	1:A:662:ARG:HD3	1.64	0.79
1:A:862:THR:CG2	1:A:864:ILE:HG12	2.12	0.79
1:A:371:THR:HG22	1:A:380:GLN:N	1.96	0.79
1:A:865:ASN:ND2	1:A:1010:PRO:HG2	1.96	0.78
1:A:587:ILE:HG23	1:A:589:ARG:NH2	2.00	0.76
1:A:302:PRO:HB2	1:A:352:ARG:HD2	1.69	0.74
1:A:107:VAL:HG23	1:A:260:TYR:CD2	2.23	0.73
1:A:620:ALA:HB2	1:A:626:ILE:HD13	1.71	0.73
1:A:862:THR:HG21	1:A:864:ILE:HG12	1.69	0.73
1:A:726:ASN:HD21	1:A:751:LYS:H	1.36	0.72
1:A:885:VAL:HG11	1:A:915:ALA:HB1	1.71	0.72
1:A:117:LEU:HD22	1:A:119:VAL:HG22	1.70	0.72
1:A:17:LYS:HA	1:A:315:GLN:HE21	1.53	0.71
1:A:839:ILE:H	1:A:839:ILE:HD13	1.55	0.71
1:A:71:GLU:HB2	1:A:93:THR:HG21	1.71	0.71
1:A:831:THR:CG2	1:A:833:PRO:HD3	2.18	0.71
1:A:289:SER:HA	1:A:657:MET:HG3	1.73	0.70
1:A:14:THR:HG23	1:A:15:TRP:O	1.91	0.70
1:A:33:VAL:HG21	1:A:115:VAL:HG23	1.72	0.70
1:A:285:GLN:NE2	1:A:617:HIS:HD2	1.85	0.70
1:A:884:GLY:HA2	1:A:896:VAL:HG13	1.74	0.70
1:A:49:HIS:CD2	1:A:373:ARG:HH12	2.09	0.69
1:A:342:LEU:HD21	1:A:398:ILE:CD1	2.22	0.69
1:A:590:LEU:HD22	1:A:632:ASP:HB3	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:LEU:HD13	1:A:238:THR:CG2	2.23	0.68
1:A:976:ILE:H	1:A:976:ILE:HD13	1.56	0.68
1:A:313:TRP:HA	1:A:315:GLN:NE2	2.02	0.67
1:A:348:GLU:HG2	1:A:352:ARG:NH1	2.10	0.67
1:A:384:GLN:NE2	1:A:430:GLU:HG2	2.10	0.67
1:A:339:THR:HG21	1:A:662:ARG:NH2	2.11	0.66
1:A:49:HIS:HD2	1:A:373:ARG:HH12	1.39	0.66
1:A:993:VAL:HB	1:A:997:GLN:HG3	1.78	0.66
1:A:348:GLU:HG2	1:A:352:ARG:HH11	1.60	0.65
1:A:948:ASP:HB3	1:A:951:TYR:HB3	1.79	0.65
1:A:560:PRO:HG2	4:A:3349:HOH:O	1.96	0.65
1:A:844:VAL:CG1	1:A:876:THR:HB	2.27	0.64
1:A:999:GLN:HA	1:A:1002:VAL:CG1	2.28	0.64
1:A:254:LYS:HA	1:A:254:LYS:HE3	1.79	0.64
1:A:429:TRP:O	1:A:431:GLU:HG3	1.98	0.64
1:A:220:LEU:HD22	1:A:226:THR:HG21	1.81	0.63
1:A:726:ASN:ND2	1:A:751:LYS:H	1.96	0.63
1:A:999:GLN:HA	1:A:1002:VAL:HG12	1.80	0.63
1:A:282:LEU:HD11	1:A:614:GLU:OE2	1.99	0.63
1:A:117:LEU:HD22	1:A:119:VAL:CG2	2.29	0.63
1:A:189:ASP:HB2	1:A:213:SER:OG	1.99	0.63
1:A:156:LEU:HD13	1:A:238:THR:HG23	1.80	0.62
1:A:324:GLU:OE2	1:A:371:THR:HG21	2.00	0.62
1:A:844:VAL:HG13	1:A:876:THR:HB	1.82	0.62
1:A:60:PHE:CE1	1:A:133:VAL:HG22	2.35	0.61
1:A:477:THR:HG22	1:A:494:TYR:OH	2.01	0.61
1:A:885:VAL:CG1	1:A:894:SER:HB3	2.30	0.60
1:A:306:ILE:HD13	1:A:306:ILE:H	1.65	0.60
1:A:587:ILE:CG2	1:A:589:ARG:NH2	2.65	0.60
1:A:49:HIS:CD2	1:A:373:ARG:HH22	2.19	0.60
1:A:220:LEU:CD2	1:A:226:THR:HG21	2.30	0.60
1:A:933:ASN:O	1:A:944:ARG:NH1	2.34	0.60
1:A:859:LEU:O	1:A:862:THR:HB	2.01	0.60
1:A:940:ILE:HG23	1:A:977:PRO:HB2	1.83	0.60
1:A:371:THR:CG2	1:A:380:GLN:H	2.01	0.60
1:A:296:HIS:O	1:A:306:ILE:HD13	2.01	0.60
1:A:965:PHE:CE1	1:A:989:LEU:HD21	2.37	0.59
1:A:336:GLN:O	1:A:339:THR:HG22	2.03	0.59
1:A:339:THR:CG2	1:A:662:ARG:HH21	2.13	0.59
1:A:107:VAL:HG21	1:A:257:SER:HA	1.84	0.59
1:A:886:TYR:CE1	1:A:892:ARG:HB2	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:ILE:HB	1:A:425:PRO:HG2	1.84	0.59
1:A:484:THR:H	1:A:504:ASN:HD21	1.49	0.59
1:A:383:ILE:HB	1:A:425:PRO:CG	2.33	0.59
1:A:218:ILE:N	1:A:218:ILE:HD12	2.17	0.58
1:A:17:LYS:HA	1:A:315:GLN:NE2	2.16	0.58
1:A:14:THR:HG21	4:A:3268:HOH:O	2.04	0.58
1:A:867:GLU:HG2	1:A:868:HIS:CE1	2.38	0.58
1:A:767:ASP:O	1:A:768:ARG:HD2	2.03	0.58
1:A:49:HIS:HD2	1:A:373:ARG:HH22	1.51	0.58
1:A:251:THR:HG22	1:A:255:LYS:HB3	1.86	0.57
1:A:566:HIS:HE1	1:A:632:ASP:OD1	1.86	0.57
1:A:862:THR:HG22	1:A:864:ILE:HG12	1.87	0.57
1:A:870:TRP:CH2	1:A:888:PRO:HA	2.40	0.57
1:A:839:ILE:HD13	1:A:839:ILE:N	2.20	0.57
1:A:76:THR:HG23	1:A:94:THR:O	2.05	0.56
1:A:929:ALA:HA	1:A:991:VAL:HG12	1.86	0.56
1:A:315:GLN:NE2	1:A:315:GLN:H	2.02	0.56
1:A:813:VAL:HG21	1:A:1018:LEU:HD21	1.86	0.56
1:A:313:TRP:CA	1:A:315:GLN:HE22	2.08	0.56
1:A:633:ARG:HD2	4:A:3105:HOH:O	2.06	0.56
1:A:777:ILE:HD11	1:A:815:ASP:HB2	1.86	0.56
1:A:335:TYR:CD1	1:A:394:LEU:HD13	2.41	0.56
1:A:507:ALA:O	1:A:520:GLU:HG3	2.05	0.56
1:A:994:GLY:O	1:A:997:GLN:HG2	2.05	0.56
1:A:112:ARG:HB2	1:A:244:THR:HG23	1.88	0.55
1:A:160:LEU:HD12	1:A:166:PRO:HB2	1.88	0.55
1:A:832:ASN:HD21	1:A:836:GLY:H	1.54	0.55
1:A:831:THR:HG22	1:A:832:ASN:N	2.22	0.55
1:A:876:THR:HG23	1:A:898:LEU:HD22	1.87	0.55
1:A:623:GLY:O	1:A:624:TYR:HB2	2.07	0.55
1:A:373:ARG:HH11	1:A:373:ARG:HG2	1.72	0.55
1:A:342:LEU:HD13	1:A:350:ALA:HB2	1.89	0.54
1:A:383:ILE:O	1:A:425:PRO:HG2	2.07	0.54
1:A:95:ASP:HB2	1:A:100:TRP:CD2	2.42	0.54
1:A:370:GLN:NE2	1:A:382:GLY:H	2.01	0.54
1:A:636:PRO:HG2	1:A:636:PRO:O	2.07	0.54
1:A:831:THR:HG22	1:A:832:ASN:H	1.72	0.54
1:A:790:PRO:HG2	1:A:792:THR:HG22	1.90	0.54
1:A:989:LEU:O	1:A:990:ASP:HB3	2.06	0.54
1:A:370:GLN:HE21	1:A:382:GLY:N	2.01	0.54
1:A:511:TRP:CE2	1:A:523:VAL:HG21	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:839:ILE:HD11	1:A:898:LEU:HD13	1.89	0.54
1:A:33:VAL:HG21	1:A:115:VAL:CG2	2.37	0.54
1:A:567:ARG:NH1	2:A:3000:ACR:O3B	2.38	0.54
1:A:916:LEU:O	1:A:918:GLY:N	2.40	0.54
1:A:977:PRO:HA	1:A:979:ARG:HH12	1.73	0.54
1:A:567:ARG:HD3	1:A:571:ASP:OD2	2.06	0.54
1:A:5:PRO:HD3	1:A:204:SER:OG	2.07	0.53
1:A:690:SER:HA	4:A:3161:HOH:O	2.06	0.53
1:A:802:VAL:CG1	1:A:803:PRO:HD2	2.39	0.53
1:A:114:THR:OG1	1:A:244:THR:HG22	2.09	0.53
1:A:335:TYR:HD1	1:A:394:LEU:HD13	1.73	0.53
1:A:268:LEU:HD21	1:A:291:MET:SD	2.48	0.53
1:A:74:GLN:HE21	1:A:95:ASP:HA	1.74	0.53
1:A:432:THR:HB	1:A:509:ARG:HH11	1.73	0.53
1:A:318:SER:HB2	1:A:320:GLU:OE2	2.07	0.53
1:A:963:TRP:O	1:A:964:ARG:HD3	2.09	0.53
1:A:440:LEU:HD23	1:A:481:MET:CE	2.38	0.53
1:A:49:HIS:HD2	1:A:373:ARG:NH1	2.05	0.53
1:A:226:THR:HG22	4:A:3244:HOH:O	2.08	0.52
1:A:1002:VAL:O	1:A:1011:VAL:HB	2.10	0.52
1:A:74:GLN:NE2	1:A:96:ASN:H	2.08	0.52
1:A:1012:VAL:O	1:A:1012:VAL:HG13	2.10	0.52
1:A:910:ARG:N	1:A:910:ARG:HD3	2.24	0.52
1:A:347:GLU:OE1	1:A:398:ILE:HG13	2.10	0.52
1:A:289:SER:CA	1:A:657:MET:HG3	2.39	0.52
1:A:862:THR:HG22	1:A:864:ILE:HG23	1.91	0.51
1:A:305:PHE:HB2	1:A:334:MET:HG3	1.91	0.51
1:A:885:VAL:HG12	1:A:894:SER:HB3	1.90	0.51
1:A:432:THR:HB	1:A:509:ARG:NH1	2.25	0.51
1:A:378:ILE:HG22	4:A:3124:HOH:O	2.10	0.51
1:A:566:HIS:CE1	1:A:590:LEU:HD13	2.46	0.51
1:A:160:LEU:HD22	1:A:160:LEU:N	2.26	0.51
1:A:833:PRO:C	1:A:835:GLY:H	2.14	0.50
1:A:826:ILE:HD11	1:A:830:VAL:HG22	1.92	0.50
1:A:147:THR:O	1:A:157:ALA:HA	2.11	0.50
1:A:479:LYS:HE2	4:A:3269:HOH:O	2.09	0.50
1:A:848:LEU:HD23	1:A:926:MET:HB3	1.93	0.50
1:A:969:ALA:HB2	1:A:1005:TRP:CH2	2.46	0.50
1:A:690:SER:O	1:A:762:GLY:HA3	2.11	0.50
1:A:338:VAL:O	1:A:342:LEU:HB2	2.12	0.50
1:A:998:THR:O	1:A:1002:VAL:HG12	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:ASP:HB2	1:A:100:TRP:CE3	2.47	0.50
1:A:511:TRP:CZ2	1:A:523:VAL:HG21	2.47	0.49
1:A:552:ASP:OD1	1:A:598:ARG:NH1	2.45	0.49
1:A:156:LEU:HD13	1:A:238:THR:HG21	1.95	0.49
1:A:484:THR:CG2	1:A:484:THR:O	2.61	0.49
1:A:58:LEU:HA	1:A:134:LEU:O	2.12	0.49
1:A:1006:ARG:HH21	1:A:1006:ARG:HG2	1.77	0.49
1:A:940:ILE:HG12	1:A:978:SER:HA	1.95	0.49
1:A:100:TRP:CD1	1:A:100:TRP:C	2.86	0.49
1:A:71:GLU:CB	1:A:93:THR:HG21	2.41	0.49
1:A:884:GLY:HA2	1:A:896:VAL:CG1	2.42	0.48
1:A:572:GLY:HA2	1:A:587:ILE:HA	1.95	0.48
1:A:946:VAL:HG22	1:A:965:PHE:HB2	1.94	0.48
1:A:998:THR:HG23	1:A:1001:ALA:H	1.79	0.48
1:A:358:PHE:CB	1:A:409:GLU:HG3	2.35	0.48
1:A:866:LEU:N	1:A:866:LEU:HD22	2.28	0.48
1:A:16:THR:CG2	1:A:38:THR:HG21	2.43	0.48
1:A:107:VAL:HG23	1:A:260:TYR:CG	2.48	0.48
1:A:62:VAL:HG11	1:A:100:TRP:CE2	2.48	0.48
1:A:952:TRP:NE1	1:A:961:LYS:HA	2.28	0.48
1:A:283:ARG:NH1	1:A:287:ASP:OD2	2.46	0.48
1:A:477:THR:CG2	1:A:494:TYR:OH	2.62	0.47
1:A:294:LYS:O	1:A:294:LYS:HD3	2.13	0.47
1:A:559:THR:HB	1:A:560:PRO:HD2	1.96	0.47
1:A:700:GLU:O	1:A:768:ARG:HG3	2.13	0.47
1:A:199:ARG:HG3	1:A:199:ARG:HH21	1.78	0.47
1:A:976:ILE:H	1:A:976:ILE:CD1	2.25	0.47
1:A:977:PRO:HA	1:A:979:ARG:NH1	2.28	0.47
1:A:610:LEU:N	1:A:611:PRO:HD2	2.30	0.47
1:A:587:ILE:HG23	1:A:589:ARG:HH21	1.79	0.47
1:A:151:THR:HB	1:A:156:LEU:HD11	1.97	0.47
1:A:659:GLN:HE22	1:A:662:ARG:HH11	1.62	0.47
1:A:107:VAL:HG22	1:A:108:THR:N	2.30	0.47
1:A:16:THR:O	1:A:314:GLY:HA3	2.15	0.46
1:A:384:GLN:HE22	1:A:430:GLU:HG2	1.78	0.46
1:A:802:VAL:HG13	1:A:803:PRO:HD2	1.98	0.46
1:A:146:ASP:O	1:A:209:PRO:HA	2.15	0.46
1:A:546:ASP:O	1:A:546:ASP:OD1	2.33	0.46
1:A:715:THR:CG2	1:A:716:THR:N	2.77	0.46
1:A:61:ALA:HA	1:A:69:GLN:O	2.15	0.46
1:A:796:PRO:HG2	1:A:801:TYR:CG	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:GLU:HB2	1:A:305:PHE:CE2	2.51	0.46
1:A:34:TRP:HB2	1:A:46:TYR:HB2	1.98	0.46
1:A:16:THR:CG2	1:A:17:LYS:N	2.79	0.46
1:A:633:ARG:HH11	1:A:633:ARG:HG3	1.81	0.46
1:A:313:TRP:CA	1:A:315:GLN:NE2	2.75	0.46
1:A:961:LYS:HG2	1:A:961:LYS:O	2.16	0.46
1:A:940:ILE:CG2	1:A:977:PRO:HB2	2.46	0.46
1:A:655:TRP:HD1	1:A:655:TRP:O	1.99	0.46
1:A:780:LEU:HB3	1:A:992:LEU:HD23	1.98	0.45
1:A:335:TYR:OH	1:A:533:ARG:NH1	2.49	0.45
1:A:837:GLN:O	1:A:839:ILE:HD13	2.17	0.45
1:A:49:HIS:HD2	1:A:373:ARG:NH2	2.13	0.45
1:A:55:THR:HG23	4:A:3279:HOH:O	2.17	0.45
1:A:179:ALA:H	1:A:217:GLN:HB3	1.82	0.45
1:A:335:TYR:O	1:A:339:THR:HB	2.17	0.45
1:A:326:TYR:CZ	2:A:3000:ACR:H7A	2.52	0.45
1:A:440:LEU:HA	1:A:443:GLN:OE1	2.17	0.45
1:A:627:PRO:HB3	1:A:651:SER:OG	2.17	0.45
1:A:861:GLY:HA3	1:A:940:ILE:O	2.17	0.45
1:A:148:GLY:HA3	1:A:182:ASN:ND2	2.31	0.45
1:A:951:TYR:CE2	1:A:971:VAL:HA	2.52	0.44
1:A:813:VAL:CG2	1:A:1018:LEU:HD21	2.47	0.44
1:A:792:THR:O	1:A:967:GLY:HA3	2.18	0.44
1:A:405:PHE:O	1:A:409:GLU:HB2	2.17	0.44
1:A:590:LEU:O	1:A:629:GLN:HA	2.18	0.44
1:A:436:SER:O	1:A:440:LEU:HB2	2.17	0.44
1:A:948:ASP:OD2	1:A:949:GLY:N	2.50	0.44
1:A:620:ALA:O	1:A:645:ARG:NH1	2.51	0.44
1:A:628:GLU:HG2	1:A:629:GLN:HG3	2.00	0.44
1:A:620:ALA:HB2	1:A:626:ILE:CD1	2.46	0.44
1:A:978:SER:C	1:A:980:ASP:H	2.20	0.44
1:A:383:ILE:HB	1:A:425:PRO:HG3	2.00	0.44
1:A:44:GLU:HG3	1:A:55:THR:O	2.17	0.44
1:A:862:THR:HG23	1:A:931:PHE:CE2	2.53	0.43
1:A:778:GLY:HA3	1:A:1018:LEU:HB3	1.99	0.43
1:A:109:ASP:HA	1:A:256:VAL:HG13	1.99	0.43
1:A:212:ILE:C	1:A:212:ILE:HD12	2.39	0.43
1:A:58:LEU:HD23	1:A:58:LEU:C	2.39	0.43
1:A:862:THR:O	1:A:863:ASN:HB2	2.18	0.43
1:A:867:GLU:HG2	1:A:868:HIS:ND1	2.33	0.43
1:A:793:TYR:HA	1:A:966:GLY:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1005:TRP:HA	1:A:1008:GLY:O	2.18	0.43
1:A:55:THR:HG22	1:A:56:ARG:N	2.34	0.43
1:A:308:SER:OG	1:A:310:THR:HG22	2.19	0.43
1:A:973:ASP:O	1:A:979:ARG:HA	2.18	0.43
1:A:699:PRO:HG2	1:A:768:ARG:HG2	2.00	0.43
1:A:467:ARG:NH1	4:A:3057:HOH:O	2.52	0.43
1:A:976:ILE:HB	1:A:977:PRO:HD2	2.01	0.43
1:A:532:VAL:HG22	4:A:3046:HOH:O	2.19	0.43
1:A:304:ALA:HB2	1:A:356:TRP:CE2	2.54	0.43
1:A:127:GLY:O	1:A:128:ASP:HB2	2.18	0.42
1:A:630:VAL:HA	1:A:645:ARG:O	2.18	0.42
1:A:973:ASP:HB2	1:A:981:THR:HG22	2.00	0.42
1:A:587:ILE:HG23	1:A:589:ARG:CZ	2.48	0.42
1:A:389:ALA:HB1	1:A:446:ALA:HB2	2.01	0.42
1:A:351:ALA:O	1:A:354:VAL:HG12	2.20	0.42
1:A:798:ASN:ND2	1:A:963:TRP:CZ2	2.87	0.42
1:A:685:ALA:HB3	4:A:3111:HOH:O	2.20	0.42
1:A:297:GLU:CD	1:A:352:ARG:HH21	2.22	0.42
1:A:74:GLN:HE21	1:A:96:ASN:H	1.68	0.42
1:A:593:LEU:HD12	1:A:593:LEU:C	2.40	0.42
1:A:417:LEU:HA	1:A:417:LEU:HD12	1.93	0.42
1:A:484:THR:HG22	1:A:484:THR:O	2.20	0.41
1:A:148:GLY:O	1:A:206:THR:HA	2.20	0.41
1:A:862:THR:HG23	1:A:931:PHE:CZ	2.54	0.41
1:A:636:PRO:CG	1:A:636:PRO:O	2.68	0.41
1:A:504:ASN:N	1:A:504:ASN:HD22	2.17	0.41
1:A:80:GLU:CD	1:A:90:ARG:HH21	2.24	0.41
1:A:49:HIS:HB3	1:A:374:VAL:HG21	2.02	0.41
1:A:90:ARG:HD3	4:A:3186:HOH:O	2.19	0.41
1:A:788:ASN:H	1:A:788:ASN:HD22	1.68	0.41
1:A:552:ASP:HA	1:A:556:SER:HB3	2.02	0.41
1:A:785:GLY:N	1:A:807:ASP:OD1	2.48	0.41
1:A:14:THR:HG21	1:A:315:GLN:O	2.21	0.41
1:A:847:TYR:O	1:A:926:MET:HA	2.20	0.41
1:A:112:ARG:HD3	1:A:244:THR:HG23	2.02	0.41
1:A:478:GLU:HG2	1:A:543:TYR:CD2	2.54	0.41
1:A:1009:SER:HA	1:A:1010:PRO:C	2.42	0.41
1:A:916:LEU:O	1:A:917:GLY:C	2.60	0.41
1:A:440:LEU:HD23	1:A:481:MET:HE2	2.02	0.41
1:A:199:ARG:HG3	1:A:199:ARG:NH2	2.35	0.41
1:A:18:GLY:HA2	1:A:310:THR:OG1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:THR:HA	4:A:3137:HOH:O	2.20	0.41
1:A:877:ASP:OD1	1:A:879:ARG:HB3	2.21	0.41
1:A:433:GLY:C	1:A:497:ILE:HD11	2.41	0.41
1:A:1002:VAL:HG13	1:A:1003:LEU:HD13	2.03	0.41
1:A:591:TRP:HA	1:A:592:PRO:HD2	1.97	0.40
1:A:440:LEU:O	1:A:444:ILE:HG13	2.22	0.40
1:A:468:ALA:HA	1:A:763:THR:OG1	2.22	0.40
1:A:315:GLN:HE21	1:A:315:GLN:H	1.67	0.40
1:A:866:LEU:HD12	1:A:927:SER:CB	2.52	0.40
1:A:310:THR:HG21	1:A:650:ALA:HA	2.03	0.40
1:A:206:THR:HG22	4:A:3215:HOH:O	2.21	0.40
1:A:788:ASN:C	1:A:788:ASN:HD22	2.24	0.40
1:A:27:LEU:HD13	1:A:27:LEU:O	2.22	0.40
1:A:181:ALA:HB3	1:A:215:THR:CG2	2.51	0.40
1:A:267:TYR:CZ	1:A:271:LEU:HD11	2.56	0.40
1:A:709:THR:HA	1:A:743:VAL:O	2.21	0.40
1:A:946:VAL:HG22	1:A:965:PHE:CB	2.52	0.40
1:A:69:GLN:OE1	1:A:100:TRP:CH2	2.75	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	1017/1020 (100%)	963 (95%)	47 (5%)	7 (1%)	26 37

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	860	PRO
1	A	917	GLY
1	A	637	THR

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Mol	Chain	Res	Type
1	A	834	TRP
1	A	835	GLY
1	A	861	GLY
1	A	686	GLY

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	752/753 (100%)	709 (94%)	43 (6%)	25	39

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	TRP
1	A	117	LEU
1	A	171	LEU
1	A	242	LEU
1	A	254	LYS
1	A	255	LYS
1	A	268	LEU
1	A	290	LEU
1	A	306	ILE
1	A	315	GLN
1	A	342	LEU
1	A	371	THR
1	A	394	LEU
1	A	398	ILE
1	A	409	GLU
1	A	410	LEU
1	A	417	LEU
1	A	427	GLU
1	A	456	LYS
1	A	495	LEU
1	A	502	ASN
1	A	524	LEU

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Mol	Chain	Res	Type
1	A	533	ARG
1	A	548	LEU
1	A	557	GLN
1	A	587	ILE
1	A	590	LEU
1	A	635	GLU
1	A	642	GLU
1	A	643	LEU
1	A	657	MET
1	A	730	THR
1	A	745	LEU
1	A	751	LYS
1	A	788	ASN
1	A	832	ASN
1	A	834	TRP
1	A	839	ILE
1	A	905	ARG
1	A	910	ARG
1	A	976	ILE
1	A	990	ASP
1	A	1018	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	HIS
1	A	74	GLN
1	A	182	ASN
1	A	214	GLN
1	A	285	GLN
1	A	315	GLN
1	A	370	GLN
1	A	408	ASN
1	A	502	ASN
1	A	504	ASN
1	A	557	GLN
1	A	566	HIS
1	A	607	GLN
1	A	617	HIS
1	A	641	HIS
1	A	659	GLN
1	A	677	GLN

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Mol	Chain	Res	Type
1	A	726	ASN
1	A	788	ASN
1	A	832	ASN
1	A	841	HIS
1	A	845	ASN
1	A	863	ASN
1	A	868	HIS
1	A	906	GLN
1	A	987	ASN
1	A	1019	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 6 are monoatomic - leaving 1 for Mogul analysis.

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	ACR	A	3000	-	33,34,47	2.10	11 (33%)	38,50,70	1.23	4 (10%)

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	ACR	A	3000	-	-	0/12/69/98	0/3/3/4

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3000	ACR	O5B-C1B	2.17	1.47	1.41
2	A	3000	ACR	C4A-C5A	2.22	1.57	1.50
2	A	3000	ACR	C3C-C4C	2.27	1.58	1.52
2	A	3000	ACR	O5C-C5C	2.44	1.48	1.43
2	A	3000	ACR	O5B-C5B	2.67	1.51	1.44
2	A	3000	ACR	C1A-N4B	2.67	1.52	1.47
2	A	3000	ACR	C1A-C7A	2.98	1.54	1.50
2	A	3000	ACR	C2C-C3C	3.20	1.56	1.52
2	A	3000	ACR	C2A-C1A	3.50	1.58	1.53
2	A	3000	ACR	C3A-C4A	4.97	1.59	1.53
2	A	3000	ACR	C7A-C5A	5.53	1.41	1.32

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3000	ACR	O4A-C4A-C3A	-2.25	105.36	109.95
2	A	3000	ACR	C1B-O4C-C4C	2.09	123.46	118.01
2	A	3000	ACR	O4C-C4C-C3C	2.52	113.67	107.17
2	A	3000	ACR	C1C-O5C-C5C	2.70	115.68	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	3000	ACR	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(Å ²)	Q<0.9
1	A	1019/1020 (99%)	0.07	56 (5%)	29 28	8, 23, 52, 76	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	959	TRP	6.1
1	A	2	THR	6.0
1	A	958	ALA	5.3
1	A	956	ASP	5.3
1	A	954	ALA	5.0
1	A	963	TRP	4.9
1	A	952	TRP	4.8
1	A	972	PHE	4.5
1	A	802	VAL	4.4
1	A	960	ILE	4.4
1	A	794	ARG	4.2
1	A	224	GLY	4.2
1	A	951	TYR	4.1
1	A	797	THR	3.9
1	A	955	GLY	3.9
1	A	687	THR	3.7
1	A	128	ASP	3.7
1	A	957	PRO	3.6
1	A	953	GLU	3.5
1	A	949	GLY	3.5
1	A	940	ILE	3.4
1	A	945	PRO	3.3
1	A	962	GLU	3.2
1	A	948	ASP	3.1
1	A	796	PRO	3.0
1	A	799	SER	2.9
1	A	975	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	880	PHE	2.7
1	A	977	PRO	2.7
1	A	947	TYR	2.7
1	A	950	ALA	2.7
1	A	834	TRP	2.7
1	A	279	THR	2.6
1	A	126	GLY	2.6
1	A	878	GLY	2.6
1	A	125	ASP	2.5
1	A	971	VAL	2.4
1	A	976	ILE	2.4
1	A	222	ALA	2.4
1	A	223	GLY	2.4
1	A	793	TYR	2.4
1	A	966	GLY	2.4
1	A	792	THR	2.4
1	A	688	PRO	2.3
1	A	817	GLY	2.3
1	A	946	VAL	2.3
1	A	123	VAL	2.2
1	A	910	ARG	2.2
1	A	322	HIS	2.2
1	A	798	ASN	2.2
1	A	818	ASP	2.2
1	A	934	ALA	2.1
1	A	841	HIS	2.1
1	A	100	TRP	2.1
1	A	833	PRO	2.1
1	A	961	LYS	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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	ACR	A	3000	32/44	0.92	0.17	3.27	15,22,43,46	0
3	CA	A	2005	1/1	0.98	0.07	-1.80	26,26,26,26	0
3	CA	A	2006	1/1	0.96	0.07	-1.91	36,36,36,36	0
3	CA	A	2001	1/1	0.96	0.08	-2.34	36,36,36,36	0
3	CA	A	2003	1/1	0.99	0.04	-4.11	27,27,27,27	0
3	CA	A	2004	1/1	0.99	0.05	-4.55	42,42,42,42	0
3	CA	A	2002	1/1	0.98	0.09	-	34,34,34,34	0

6.5 Other polymers

There are no such residues in this entry.