Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:53 PM GMT

PDB ID	:	1R0K
Title	:	Crystal structure of 1-deoxy-D-xylulose 5-phosphate reductoisomerase from Zymomonas mobilis
Authors	:	Ricagno, S.; Grolle, S.; Bringer-Meyer, S.; Sahm, H.; Lindqvist, Y.; Schneider, G.
Deposited on	:	2003-09-22
Resolution	:	1.91 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 (1)) were used in the production of this report:

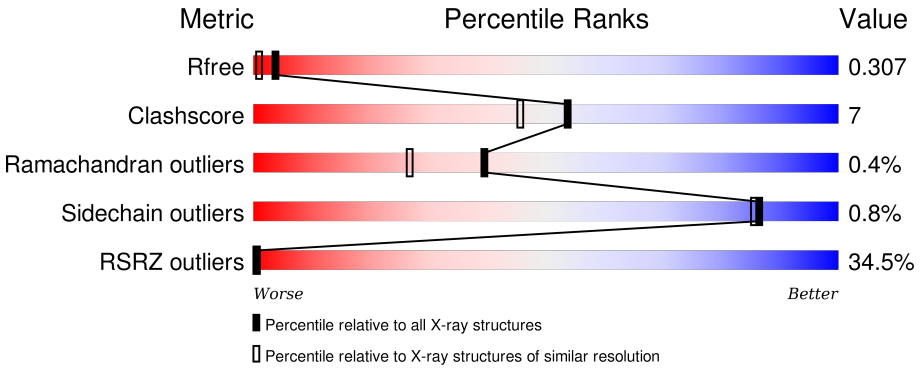
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.91 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	5832 (1.94-1.90)
Clashscore	102246	6540 (1.94-1.90)
Ramachandran outliers	100387	6464 (1.94-1.90)
Sidechain outliers	100360	6465 (1.94-1.90)
RSRZ outliers	91569	5846 (1.94-1.90)

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	388	60% 85% 13% •
1	B	388	25% 87% 11% ••
1	C	388	28% 82% 15% ••
1	D	388	22% 81% 17% ••

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ACT	C	1303	-	-	-	X

2 Entry composition

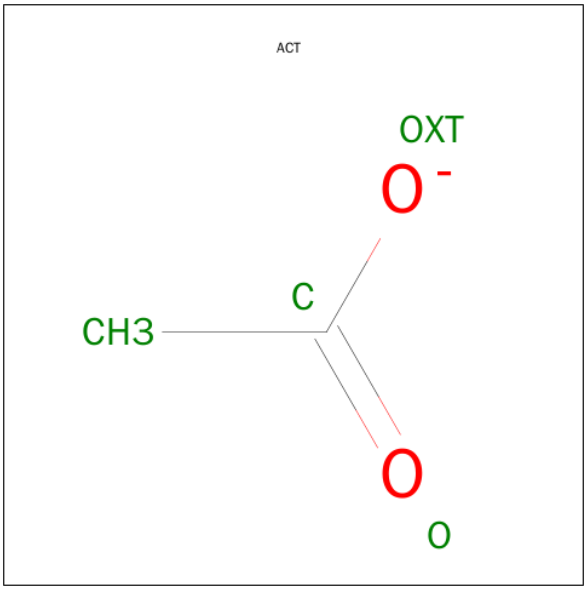
There are 3 unique types of molecules in this entry. The entry contains 12721 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 1-deoxy-D-xylulose 5-phosphate reductoisomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	380	Total	C	N	O	S	0	0	0
			2867	1806	498	547	16			
1	B	382	Total	C	N	O	S	0	0	0
			2885	1817	502	549	17			
1	C	379	Total	C	N	O	S	0	0	0
			2858	1801	496	545	16			
1	D	380	Total	C	N	O	S	0	0	0
			2871	1808	500	546	17			

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0

- Molecule 3 is water.

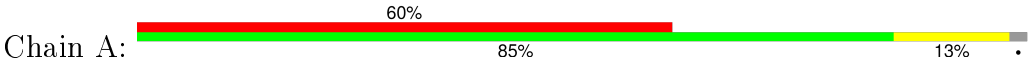
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	297	Total O 297 297	0	0
3	B	349	Total O 349 349	0	0
3	C	291	Total O 291 291	0	0
3	D	287	Total O 287 287	0	0

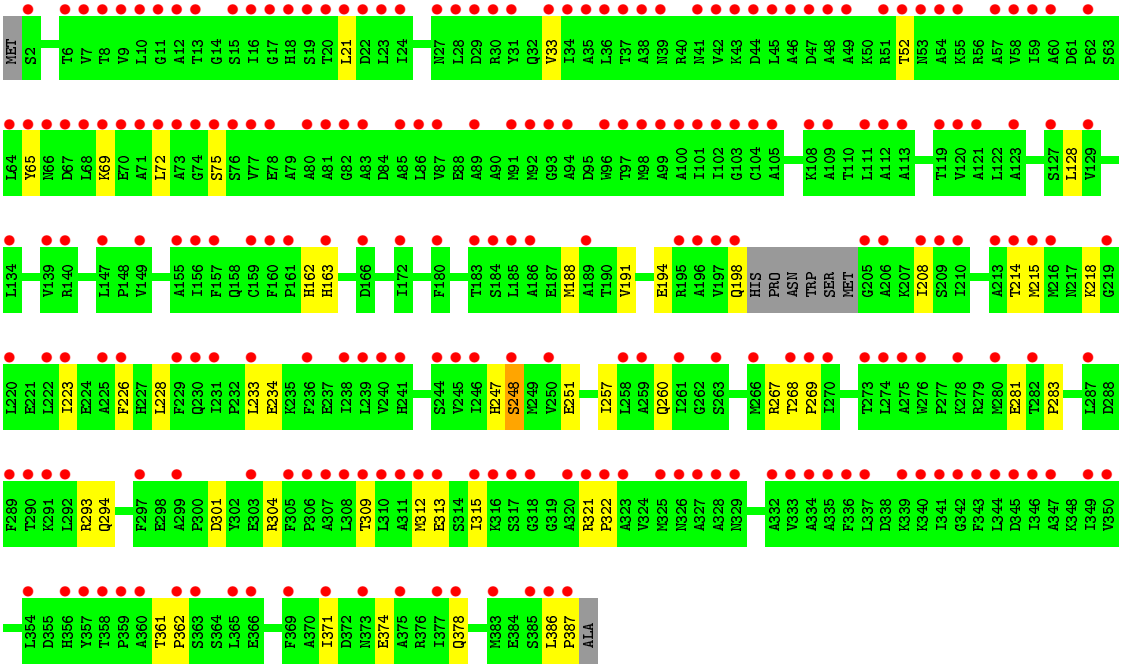
3 Residue-property plots (i)

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: 1-deoxy-D-xylulose 5-phosphate reductoisomerase

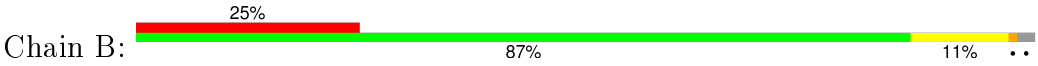
Chain A:

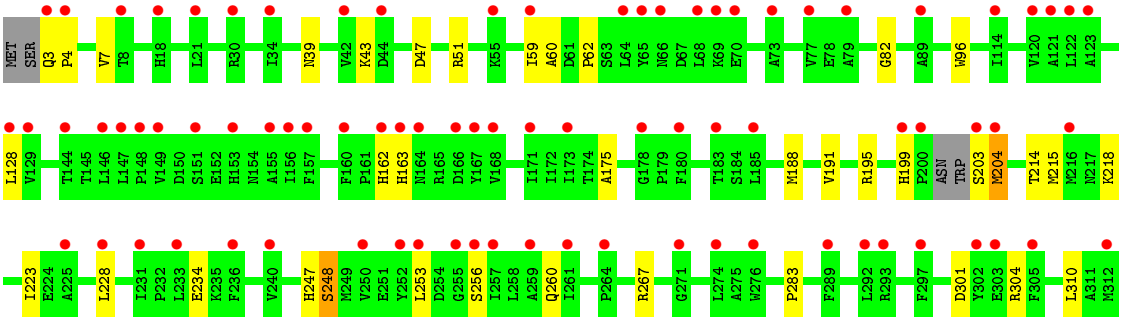


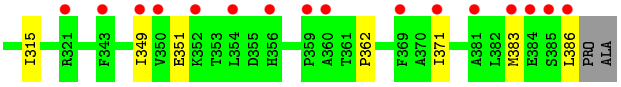


- Molecule 1: 1-deoxy-D-xylulose 5-phosphate reductoisomerase

Chain B:

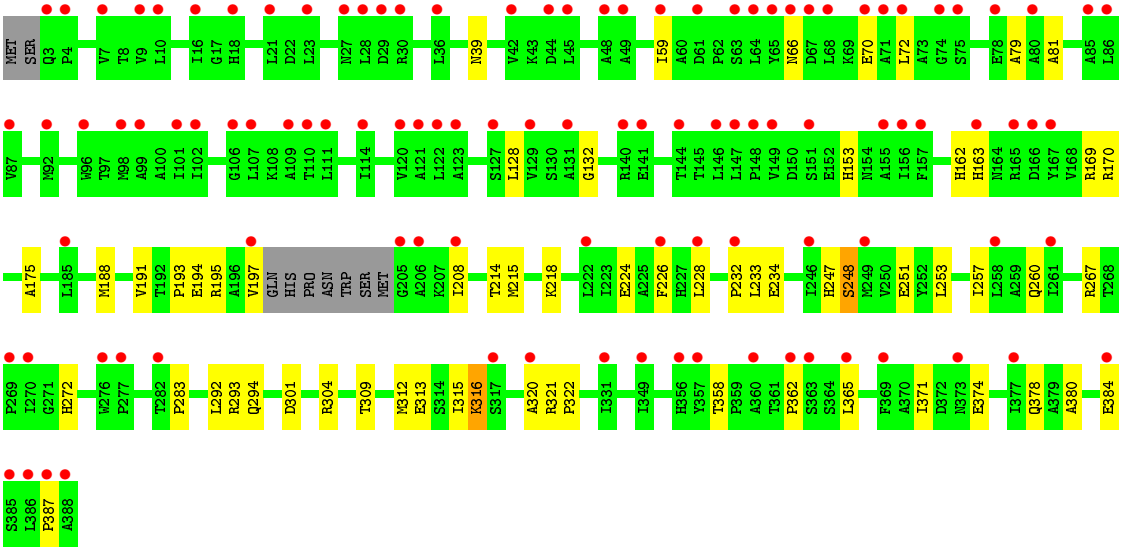






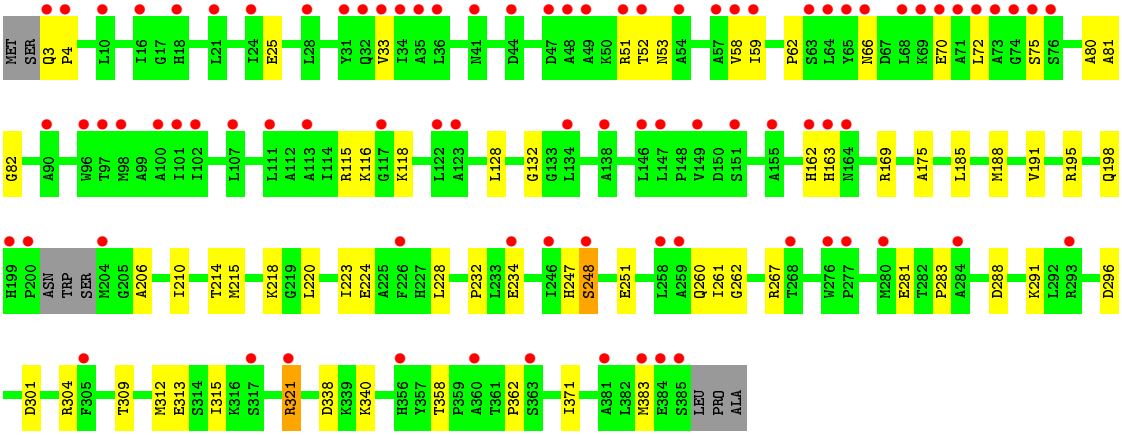
• Molecule 1: 1-deoxy-D-xylulose 5-phosphate reductoisomerase

Chain C:



• Molecule 1: 1-deoxy-D-xylulose 5-phosphate reductoisomerase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	87.70Å 93.20Å 98.60Å 90.00° 90.50° 90.00°	Depositor
Resolution (Å)	29.63 – 1.91 29.63 – 1.91	Depositor EDS
% Data completeness (in resolution range)	95.9 (29.63-1.91) 95.9 (29.63-1.91)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.29 (at 1.91Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.200 , 0.230 0.294 , 0.307	Depositor DCC
R_{free} test set	2810 reflections (2.43%)	DCC
Wilson B-factor (Å^2)	16.7	Xtriage
Anisotropy	0.669	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 52.4	EDS
Estimated twinning fraction	0.000 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Outliers	3 of 118460 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	12721	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 52.11 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 5.0945e-05.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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

5.1 Standard geometry

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

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	0.29	0/2915	0.55	0/3953
1	B	0.29	0/2934	0.55	0/3978
1	C	0.29	0/2906	0.56	0/3940
1	D	0.29	0/2920	0.55	0/3959
All	All	0.29	0/11675	0.55	0/15830

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

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	2867	0	2903	34	0
1	B	2885	0	2919	31	0
1	C	2858	0	2895	43	0
1	D	2871	0	2903	46	0
2	A	4	0	3	0	0
2	B	4	0	3	0	0
2	C	4	0	3	1	0
2	D	4	0	3	0	0
3	A	297	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	349	0	0	2	1
3	C	291	0	0	3	1
3	D	287	0	0	6	0
All	All	12721	0	11632	151	1

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 7.

All (151) 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:362:PRO:HG3	1:A:371:ILE:HD12	1.63	0.81
1:C:362:PRO:HG3	1:C:371:ILE:HD12	1.63	0.80
1:D:66:ASN:O	1:D:70:GLU:HG3	1.87	0.73
1:B:234:GLU:H	1:B:234:GLU:CD	1.93	0.73
1:D:234:GLU:CD	1:D:234:GLU:H	1.92	0.72
1:D:185:LEU:HD23	1:D:188:MET:HE3	1.70	0.72
1:C:301:ASP:OD2	1:C:304:ARG:HD3	1.90	0.70
1:B:267:ARG:CZ	1:B:283:PRO:HG2	2.22	0.69
1:C:233:LEU:HD13	1:C:312:MET:HE1	1.75	0.68
1:C:321:ARG:HB2	1:C:322:PRO:HD3	1.75	0.68
1:D:3:GLN:HB3	1:D:4:PRO:HA	1.75	0.68
1:A:321:ARG:HB2	1:A:322:PRO:HD3	1.77	0.67
1:A:234:GLU:CD	1:A:234:GLU:H	1.97	0.66
1:D:321:ARG:HG2	1:D:321:ARG:HH11	1.61	0.66
1:A:386:LEU:HD12	1:A:387:PRO:HD2	1.78	0.66
1:C:234:GLU:CD	1:C:234:GLU:H	1.99	0.65
1:C:267:ARG:CZ	1:C:283:PRO:HG2	2.25	0.65
1:D:267:ARG:CZ	1:D:283:PRO:HG2	2.29	0.63
1:B:199:HIS:HE2	1:B:203:SER:N	1.96	0.62
1:C:293:ARG:HG2	1:C:294:GLN:HG3	1.81	0.62
1:B:362:PRO:HG3	1:B:371:ILE:HD12	1.80	0.62
1:B:362:PRO:HG3	1:B:371:ILE:CD1	2.32	0.60
1:B:43:LYS:HE2	1:B:47:ASP:OD2	2.02	0.60
1:B:386:LEU:O	1:B:386:LEU:HD23	2.03	0.59
1:C:208:ILE:HG12	3:C:1559:HOH:O	2.02	0.58
1:A:301:ASP:OD2	1:A:304:ARG:HD3	2.01	0.58
1:D:301:ASP:OD2	1:D:304:ARG:HD3	2.04	0.58
1:D:312:MET:HE1	3:D:1552:HOH:O	2.04	0.58
1:C:309:THR:O	1:C:313:GLU:HG3	2.03	0.57
1:B:267:ARG:NH1	1:B:283:PRO:HG2	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:321:ARG:HH21	1:D:358:THR:HG21	1.69	0.56
1:C:380:ALA:O	1:C:384:GLU:HG2	2.05	0.56
1:D:383:MET:HE3	3:D:1571:HOH:O	2.06	0.56
1:A:65:TYR:CZ	1:A:69:LYS:HD2	2.41	0.55
1:A:309:THR:O	1:A:313:GLU:HG3	2.06	0.55
1:D:116:LYS:HG3	3:D:1355:HOH:O	2.07	0.55
1:D:25:GLU:OE1	1:D:51:ARG:HD3	2.06	0.55
1:D:321:ARG:HH21	1:D:358:THR:CG2	2.19	0.55
1:B:47:ASP:O	1:B:51:ARG:HG3	2.07	0.54
1:D:188:MET:HA	1:D:191:VAL:HG23	1.90	0.54
1:A:267:ARG:CZ	1:A:283:PRO:HG2	2.38	0.54
1:D:72:LEU:O	1:D:75:SER:HB3	2.09	0.53
1:D:362:PRO:HG3	1:D:371:ILE:HD12	1.91	0.53
1:D:288:ASP:CG	1:D:291:LYS:HG2	2.30	0.53
1:B:203:SER:O	1:B:204:MET:O	2.27	0.52
1:A:72:LEU:O	1:A:75:SER:HB3	2.08	0.52
1:D:309:THR:O	1:D:313:GLU:HG3	2.10	0.52
1:A:226:PHE:CD2	1:A:315:ILE:HD11	2.45	0.52
1:D:267:ARG:NH1	1:D:283:PRO:HG2	2.25	0.52
1:D:128:LEU:HD13	1:D:228:LEU:HG	1.92	0.51
1:A:162:HIS:O	1:A:163:HIS:HB2	2.11	0.51
1:C:128:LEU:HD13	1:C:228:LEU:HG	1.92	0.51
1:D:232:PRO:HB3	1:D:234:GLU:OE2	2.10	0.51
1:D:321:ARG:HE	1:D:358:THR:HG22	1.75	0.51
1:B:301:ASP:OD2	1:B:304:ARG:HD3	2.11	0.50
1:C:188:MET:O	1:C:191:VAL:HG22	2.11	0.50
1:B:7:VAL:HG12	1:B:96:TRP:HB3	1.93	0.50
1:D:198:GLN:OE1	1:D:198:GLN:HA	2.11	0.50
1:A:188:MET:O	1:A:191:VAL:HG22	2.12	0.50
1:A:312:MET:HE3	1:A:315:ILE:HG23	1.94	0.49
1:C:193:PRO:HD2	1:C:194:GLU:OE2	2.11	0.49
1:A:208:ILE:HG12	3:A:1383:HOH:O	2.11	0.49
1:C:233:LEU:HD13	1:C:312:MET:CE	2.41	0.49
1:D:362:PRO:HG3	1:D:371:ILE:CD1	2.42	0.48
1:C:272:HIS:HB2	3:D:1469:HOH:O	2.13	0.48
1:D:220:LEU:O	1:D:224:GLU:HG3	2.12	0.48
1:D:223:ILE:HA	1:D:315:ILE:HD11	1.94	0.48
1:D:338:ASP:OD1	1:D:340:LYS:HE3	2.13	0.48
1:A:65:TYR:CE2	1:A:69:LYS:HD2	2.48	0.48
1:A:214:THR:O	1:A:215:MET:HB2	2.13	0.48
1:A:233:LEU:HD13	1:A:312:MET:CE	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:214:THR:O	1:C:215:MET:HB2	2.14	0.47
1:A:194:GLU:O	1:A:198:GLN:HB2	2.14	0.47
1:A:362:PRO:HG3	1:A:371:ILE:CD1	2.36	0.47
1:C:320:ALA:HB1	1:C:371:ILE:HD13	1.96	0.47
1:A:33:VAL:HG21	1:A:52:THR:HB	1.97	0.47
1:A:233:LEU:HD13	1:A:312:MET:HE3	1.96	0.47
1:C:72:LEU:HD12	1:C:79:ALA:HB2	1.97	0.47
1:D:206:ALA:O	1:D:210:ILE:HG12	2.15	0.47
1:D:59:ILE:O	1:D:81:ALA:HA	2.15	0.46
1:D:118:LYS:HE3	3:D:1457:HOH:O	2.15	0.46
1:B:62:PRO:HG3	1:B:82:GLY:HA2	1.97	0.46
1:C:253:LEU:HD13	1:D:281:GLU:HG2	1.97	0.46
1:B:162:HIS:O	1:B:163:HIS:HB2	2.15	0.46
1:C:312:MET:O	1:C:312:MET:HE3	2.15	0.46
1:B:214:THR:O	1:B:215:MET:HB2	2.15	0.46
1:C:226:PHE:CD2	1:C:315:ILE:HD11	2.51	0.46
1:C:162:HIS:O	1:C:163:HIS:HB2	2.16	0.46
1:D:33:VAL:HG21	1:D:52:THR:HB	1.98	0.45
1:D:214:THR:O	1:D:215:MET:HB2	2.16	0.45
1:C:169:ARG:HD2	1:C:251:GLU:OE2	2.16	0.45
1:D:169:ARG:HD2	1:D:251:GLU:OE2	2.16	0.45
1:C:294:GLN:HG2	1:D:296:ASP:OD1	2.17	0.45
1:B:256:SER:HB2	3:B:1422:HOH:O	2.17	0.45
1:C:321:ARG:CB	1:C:322:PRO:HD3	2.45	0.45
1:B:267:ARG:NH1	1:B:283:PRO:CG	2.79	0.45
1:C:251:GLU:HG3	1:C:257:ILE:HG12	1.99	0.44
1:C:66:ASN:O	1:C:70:GLU:HG3	2.17	0.44
1:B:223:ILE:HG12	1:B:315:ILE:CG1	2.48	0.44
1:D:321:ARG:NH1	1:D:321:ARG:HG2	2.30	0.44
1:A:251:GLU:HG3	1:A:257:ILE:HG12	1.99	0.44
1:C:316:LYS:HD2	3:C:1564:HOH:O	2.18	0.44
1:B:199:HIS:HB3	3:B:1577:HOH:O	2.17	0.44
1:C:267:ARG:NH1	1:C:283:PRO:HG2	2.34	0.43
1:D:115:ARG:HD2	3:D:1522:HOH:O	2.18	0.43
1:B:234:GLU:CD	1:B:234:GLU:N	2.68	0.43
1:C:128:LEU:HA	1:C:132:GLY:HA2	2.00	0.43
1:D:175:ALA:HA	1:D:218:LYS:HE3	2.01	0.43
1:D:162:HIS:O	1:D:163:HIS:HB2	2.18	0.43
1:C:292:LEU:O	1:C:293:ARG:HB3	2.18	0.43
1:D:58:VAL:HG22	1:D:80:ALA:HB3	2.00	0.43
1:C:175:ALA:CB	1:C:218:LYS:HE3	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:ILE:HG12	1:A:315:ILE:HB	2.01	0.43
1:D:128:LEU:HA	1:D:132:GLY:HA2	2.01	0.43
1:D:185:LEU:HD23	1:D:188:MET:CE	2.43	0.43
1:B:39:ASN:HA	1:B:60:ALA:HB3	2.01	0.43
1:B:128:LEU:HD13	1:B:228:LEU:HG	2.01	0.42
1:B:59:ILE:O	1:B:59:ILE:HG23	2.19	0.42
1:A:128:LEU:HD13	1:A:228:LEU:HG	2.00	0.42
1:C:39:ASN:HB3	2:C:1303:ACT:C	2.50	0.42
1:C:218:LYS:HA	1:C:218:LYS:HD3	1.81	0.42
1:B:3:GLN:HG2	1:B:4:PRO:HD2	2.01	0.42
1:D:62:PRO:HG3	1:D:82:GLY:HA2	2.00	0.42
1:C:193:PRO:O	1:C:197:VAL:HG22	2.19	0.42
1:C:59:ILE:O	1:C:81:ALA:HA	2.19	0.42
1:C:153:HIS:CE1	1:C:224:GLU:HB2	2.55	0.42
1:D:261:ILE:HG22	1:D:262:GLY:N	2.35	0.42
1:B:175:ALA:HA	1:B:218:LYS:HE3	2.02	0.42
1:C:358:THR:HG22	3:C:1435:HOH:O	2.19	0.42
1:D:247:HIS:O	1:D:248:SER:CB	2.68	0.41
1:A:223:ILE:HG23	1:A:315:ILE:HD13	2.02	0.41
1:D:3:GLN:HB3	1:D:4:PRO:CA	2.45	0.41
1:B:310:LEU:HD21	1:B:351:GLU:HG3	2.01	0.41
1:B:223:ILE:HA	1:B:315:ILE:HD11	2.03	0.41
1:B:188:MET:HA	1:B:191:VAL:HG23	2.03	0.41
1:A:321:ARG:CB	1:A:322:PRO:HD3	2.49	0.41
1:C:232:PRO:HB3	1:C:234:GLU:OE2	2.20	0.41
1:B:349:ILE:HD12	1:B:383:MET:HA	2.03	0.41
1:A:218:LYS:HD3	1:A:218:LYS:HA	1.82	0.41
1:A:21:LEU:HD23	1:A:21:LEU:HA	1.96	0.41
1:C:247:HIS:O	1:C:248:SER:CB	2.68	0.41
1:A:361:THR:HA	1:A:362:PRO:HD3	1.89	0.41
1:A:247:HIS:O	1:A:248:SER:CB	2.68	0.41
1:A:268:THR:HB	1:A:269:PRO:CD	2.51	0.41
1:A:374:GLU:O	1:A:378:GLN:HG2	2.21	0.41
1:B:247:HIS:O	1:B:248:SER:CB	2.69	0.40
1:C:170:ARG:NE	1:C:251:GLU:OE1	2.46	0.40
1:A:293:ARG:HG2	1:A:294:GLN:HG3	2.02	0.40
1:C:374:GLU:O	1:C:378:GLN:HG2	2.21	0.40
1:C:365:LEU:HD23	1:C:365:LEU:HA	1.93	0.40
1:A:281:GLU:HG2	1:B:253:LEU:HB3	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1567:HOH:O	3:C:1473:HOH:O[2_655]	2.07	0.13

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	376/388 (97%)	367 (98%)	8 (2%)	1 (0%)	46	34
1	B	378/388 (97%)	367 (97%)	9 (2%)	2 (0%)	34	20
1	C	375/388 (97%)	360 (96%)	13 (4%)	2 (0%)	34	20
1	D	376/388 (97%)	367 (98%)	8 (2%)	1 (0%)	46	34
All	All	1505/1552 (97%)	1461 (97%)	38 (2%)	6 (0%)	39	27

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	204	MET
1	A	248	SER
1	B	248	SER
1	C	248	SER
1	D	248	SER
1	C	387	PRO

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	301/308 (98%)	300 (100%)	1 (0%)	94 95
1	B	303/308 (98%)	301 (99%)	2 (1%)	88 88
1	C	299/308 (97%)	296 (99%)	3 (1%)	82 80
1	D	301/308 (98%)	297 (99%)	4 (1%)	76 73
All	All	1204/1232 (98%)	1194 (99%)	10 (1%)	86 85

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	260	GLN
1	B	195	ARG
1	B	260	GLN
1	C	195	ARG
1	C	260	GLN
1	C	316	LYS
1	D	53	ASN
1	D	195	ARG
1	D	260	GLN
1	D	321	ARG

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

Mol	Chain	Res	Type
1	A	53	ASN
1	A	66	ASN
1	A	260	GLN
1	B	53	ASN
1	B	142	HIS
1	B	227	HIS
1	B	260	GLN
1	C	53	ASN
1	C	142	HIS
1	C	260	GLN
1	D	53	ASN
1	D	260	GLN

5.3.3 RNA

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)

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	ACT	A	1301	-	1,3,3	0.96	0	0,3,3	0.00	-
2	ACT	B	1302	-	1,3,3	0.82	0	0,3,3	0.00	-
2	ACT	C	1303	-	1,3,3	0.80	0	0,3,3	0.00	-
2	ACT	D	1304	-	1,3,3	1.05	0	0,3,3	0.00	-

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	ACT	A	1301	-	-	0/0/0/0	0/0/0/0
2	ACT	B	1302	-	-	0/0/0/0	0/0/0/0
2	ACT	C	1303	-	-	0/0/0/0	0/0/0/0
2	ACT	D	1304	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

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	C	1303	ACT	1	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, 95^{th} 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	380/388 (97%)	2.37	233 (61%) 0 0	8, 18, 33, 53	0
1	B	382/388 (98%)	1.62	98 (25%) 1 1	9, 17, 34, 57	0
1	C	379/388 (97%)	1.65	107 (28%) 1 1	10, 18, 33, 56	0
1	D	380/388 (97%)	1.49	86 (22%) 1 1	10, 19, 34, 62	0
All	All	1521/1552 (98%)	1.78	524 (34%) 0 0	8, 18, 33, 62	0

All (524) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	386	LEU	9.3
1	D	3	GLN	7.7
1	A	198	GLN	6.7
1	B	3	GLN	6.7
1	C	387	PRO	6.4
1	A	386	LEU	6.2
1	C	386	LEU	6.2
1	A	387	PRO	6.1
1	B	203	SER	5.3
1	A	65	TYR	5.3
1	C	388	ALA	5.2
1	A	24	ILE	5.2
1	A	358	THR	4.9
1	D	4	PRO	4.8
1	C	356	HIS	4.7
1	D	385	SER	4.7
1	A	77	VAL	4.5
1	A	71	ALA	4.3
1	A	73	ALA	4.3
1	A	81	ALA	4.3
1	C	365	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
1	D	163	HIS	4.2
1	D	384	GLU	4.2
1	C	65	TYR	4.2
1	A	49	ALA	4.2
1	C	205	GLY	4.2
1	A	20	THR	4.1
1	A	72	LEU	4.1
1	C	61	ASP	4.0
1	B	70	GLU	4.0
1	C	30	ARG	4.0
1	A	197	VAL	4.0
1	C	18	HIS	4.0
1	D	73	ALA	4.0
1	A	2	SER	3.9
1	A	86	LEU	3.9
1	A	336	PHE	3.9
1	B	73	ALA	3.9
1	B	256	SER	3.9
1	A	58	VAL	3.8
1	C	29	ASP	3.8
1	A	328	ALA	3.8
1	C	149	VAL	3.8
1	A	75	SER	3.8
1	A	369	PHE	3.8
1	D	71	ALA	3.8
1	B	204	MET	3.8
1	B	163	HIS	3.7
1	C	122	LEU	3.7
1	A	339	LYS	3.7
1	A	64	LEU	3.7
1	A	104	CYS	3.7
1	A	69	LYS	3.7
1	A	357	TYR	3.7
1	A	54	ALA	3.6
1	A	91	MET	3.6
1	B	180	PHE	3.6
1	A	270	ILE	3.6
1	A	308	LEU	3.6
1	C	68	LEU	3.6
1	A	48	ALA	3.6
1	C	71	ALA	3.6
1	A	385	SER	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	23	LEU	3.6
1	A	87	VAL	3.6
1	A	28	LEU	3.5
1	A	35	ALA	3.5
1	A	213	ALA	3.5
1	A	30	ARG	3.5
1	A	349	ILE	3.5
1	B	200	PRO	3.5
1	B	128	LEU	3.5
1	B	255	GLY	3.5
1	C	360	ALA	3.5
1	A	229	PHE	3.5
1	A	365	LEU	3.5
1	B	383	MET	3.5
1	A	189	ALA	3.5
1	A	36	LEU	3.5
1	A	205	GLY	3.4
1	A	209	SER	3.4
1	D	75	SER	3.4
1	A	210	ILE	3.4
1	C	99	ALA	3.4
1	A	244	SER	3.4
1	A	220	LEU	3.4
1	B	233	LEU	3.4
1	A	51	ARG	3.4
1	B	69	LYS	3.4
1	A	34	ILE	3.4
1	A	157	PHE	3.4
1	C	369	PHE	3.4
1	A	96	TRP	3.4
1	A	216	MET	3.4
1	B	354	LEU	3.4
1	A	33	VAL	3.3
1	A	359	PRO	3.3
1	A	335	ALA	3.3
1	D	65	TYR	3.3
1	B	4	PRO	3.3
1	A	317	SER	3.3
1	A	261	ILE	3.3
1	D	101	ILE	3.3
1	A	274	LEU	3.2
1	A	12	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	123	ALA	3.2
1	B	167	TYR	3.2
1	A	6	THR	3.2
1	A	37	THR	3.2
1	A	226	PHE	3.2
1	A	21	LEU	3.2
1	A	80	ALA	3.2
1	A	163	HIS	3.2
1	B	122	LEU	3.2
1	D	356	HIS	3.2
1	A	27	ASN	3.2
1	A	318	GLY	3.2
1	C	362	PRO	3.2
1	D	277	PRO	3.2
1	A	383	MET	3.2
1	D	164	ASN	3.2
1	A	101	ILE	3.2
1	A	42	VAL	3.2
1	C	75	SER	3.2
1	A	38	ALA	3.2
1	A	60	ALA	3.2
1	A	183	THR	3.2
1	B	384	GLU	3.2
1	D	28	LEU	3.2
1	C	357	TYR	3.1
1	D	146	LEU	3.1
1	D	383	MET	3.1
1	A	222	LEU	3.1
1	A	160	PHE	3.1
1	A	282	THR	3.1
1	A	46	ALA	3.1
1	A	129	VAL	3.1
1	C	131	ALA	3.1
1	A	184	SER	3.1
1	A	315	ILE	3.1
1	D	48	ALA	3.1
1	A	195	ARG	3.1
1	A	236	PHE	3.1
1	A	83	ALA	3.1
1	A	362	PRO	3.1
1	B	303	GLU	3.1
1	A	18	HIS	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	97	THR	3.0
1	A	45	LEU	3.0
1	A	111	LEU	3.0
1	C	64	LEU	3.0
1	B	160	PHE	3.0
1	A	245	VAL	3.0
1	C	148	PRO	3.0
1	C	72	LEU	3.0
1	D	258	LEU	3.0
1	C	120	VAL	3.0
1	A	8	THR	3.0
1	A	375	ALA	3.0
1	A	93	GLY	3.0
1	A	346	ILE	3.0
1	C	109	ALA	2.9
1	C	163	HIS	2.9
1	A	140	ARG	2.9
1	A	206	ALA	2.9
1	A	230	GLN	2.9
1	C	86	LEU	2.9
1	A	208	ILE	2.9
1	D	276	TRP	2.9
1	C	7	VAL	2.9
1	C	385	SER	2.9
1	A	360	ALA	2.9
1	D	199	HIS	2.9
1	A	354	LEU	2.9
1	C	140	ARG	2.9
1	A	149	VAL	2.9
1	C	49	ALA	2.9
1	B	305	PHE	2.9
1	B	356	HIS	2.9
1	A	62	PRO	2.9
1	A	258	LEU	2.9
1	D	72	LEU	2.9
1	D	24	ILE	2.9
1	A	7	VAL	2.9
1	C	85	ALA	2.9
1	B	302	TYR	2.9
1	A	305	PHE	2.8
1	C	102	ILE	2.8
1	B	120	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	68	LEU	2.8
1	A	219	GLY	2.8
1	B	79	ALA	2.8
1	A	9	VAL	2.8
1	A	119	THR	2.8
1	A	312	MET	2.8
1	A	307	ALA	2.8
1	B	123	ALA	2.8
1	A	238	ILE	2.8
1	A	67	ASP	2.8
1	A	159	CYS	2.8
1	D	47	ASP	2.8
1	A	321	ARG	2.8
1	D	54	ALA	2.8
1	A	350	VAL	2.8
1	C	87	VAL	2.8
1	A	344	LEU	2.7
1	D	52	THR	2.7
1	A	356	HIS	2.7
1	C	197	VAL	2.7
1	A	31	TYR	2.7
1	A	322	PRO	2.7
1	A	39	ASN	2.7
1	A	373	ASN	2.7
1	A	290	THR	2.7
1	B	199	HIS	2.7
1	C	208	ILE	2.7
1	D	34	ILE	2.7
1	A	120	VAL	2.7
1	A	17	GLY	2.7
1	C	21	LEU	2.7
1	B	168	VAL	2.7
1	B	18	HIS	2.7
1	A	273	THR	2.7
1	B	155	ALA	2.7
1	C	320	ALA	2.7
1	C	96	TRP	2.7
1	A	102	ILE	2.7
1	A	52	THR	2.7
1	A	57	ALA	2.7
1	A	280	MET	2.7
1	B	65	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	310	LEU	2.7
1	A	240	VAL	2.6
1	A	309	THR	2.6
1	B	149	VAL	2.6
1	A	334	ALA	2.6
1	B	381	ALA	2.6
1	D	57	ALA	2.6
1	A	127	SER	2.6
1	B	264	PRO	2.6
1	A	291	LYS	2.6
1	D	134	LEU	2.6
1	C	166	ASP	2.6
1	A	377	ILE	2.6
1	B	231	ILE	2.6
1	D	18	HIS	2.6
1	B	164	ASN	2.6
1	C	10	LEU	2.6
1	D	21	LEU	2.6
1	D	64	LEU	2.6
1	A	13	THR	2.6
1	A	196	ALA	2.6
1	B	156	ILE	2.6
1	C	156	ILE	2.6
1	A	53	ASN	2.6
1	B	157	PHE	2.6
1	B	312	MET	2.6
1	D	70	GLU	2.6
1	A	41	ASN	2.6
1	A	161	PRO	2.6
1	D	44	ASP	2.6
1	A	74	GLY	2.6
1	A	172	ILE	2.6
1	A	76	SER	2.6
1	B	185	LEU	2.6
1	A	89	ALA	2.6
1	D	51	ARG	2.6
1	A	215	MET	2.5
1	C	92	MET	2.5
1	D	66	ASN	2.5
1	A	78	GLU	2.5
1	B	343	PHE	2.5
1	D	305	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	129	VAL	2.5
1	A	341	ILE	2.5
1	B	385	SER	2.5
1	B	55	LYS	2.5
1	A	306	PRO	2.5
1	A	292	LEU	2.5
1	C	228	LEU	2.5
1	C	78	GLU	2.5
1	A	15	SER	2.5
1	A	214	THR	2.5
1	B	349	ILE	2.5
1	C	101	ILE	2.5
1	A	98	MET	2.5
1	D	381	ALA	2.5
1	A	329	ASN	2.5
1	A	233	LEU	2.5
1	C	146	LEU	2.5
1	A	297	PHE	2.5
1	B	369	PHE	2.5
1	A	92	MET	2.5
1	A	342	GLY	2.5
1	A	316	LYS	2.5
1	A	22	ASP	2.5
1	B	114	ILE	2.5
1	C	67	ASP	2.5
1	A	299	ALA	2.5
1	B	297	PHE	2.5
1	D	58	VAL	2.5
1	A	105	ALA	2.5
1	A	44	ASP	2.5
1	D	122	LEU	2.5
1	A	29	ASP	2.4
1	A	103	GLY	2.4
1	B	30	ARG	2.4
1	A	325	MET	2.4
1	A	276	TRP	2.4
1	B	42	VAL	2.4
1	B	44	ASP	2.4
1	A	223	ILE	2.4
1	A	259	ALA	2.4
1	A	275	ALA	2.4
1	A	332	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	293	ARG	2.4
1	D	102	ILE	2.4
1	D	200	PRO	2.4
1	C	111	LEU	2.4
1	A	347	ALA	2.4
1	C	155	ALA	2.4
1	A	269	PRO	2.4
1	B	173	ILE	2.4
1	B	183	THR	2.4
1	B	64	LEU	2.4
1	B	68	LEU	2.4
1	C	107	LEU	2.4
1	C	147	LEU	2.4
1	A	139	VAL	2.4
1	B	250	VAL	2.4
1	D	149	VAL	2.4
1	A	155	ALA	2.4
1	C	165	ARG	2.4
1	A	248	SER	2.4
1	C	270	ILE	2.4
1	C	373	ASN	2.4
1	C	222	LEU	2.4
1	C	121	ALA	2.4
1	B	289	PHE	2.4
1	C	246	ILE	2.3
1	D	321	ARG	2.3
1	A	239	LEU	2.3
1	B	253	LEU	2.3
1	C	258	LEU	2.3
1	C	232	PRO	2.3
1	B	121	ALA	2.3
1	C	48	ALA	2.3
1	D	259	ALA	2.3
1	D	33	VAL	2.3
1	C	74	GLY	2.3
1	D	74	GLY	2.3
1	C	276	TRP	2.3
1	A	10	LEU	2.3
1	A	185	LEU	2.3
1	A	287	LEU	2.3
1	B	228	LEU	2.3
1	D	68	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	112	ALA	2.3
1	B	225	ALA	2.3
1	D	155	ALA	2.3
1	A	156	ILE	2.3
1	B	371	ILE	2.3
1	C	261	ILE	2.3
1	B	252	TYR	2.3
1	C	151	SER	2.3
1	A	225	ALA	2.3
1	A	327	ALA	2.3
1	A	337	LEU	2.3
1	C	23	LEU	2.3
1	C	45	LEU	2.3
1	D	100	ALA	2.3
1	A	11	GLY	2.3
1	D	204	MET	2.3
1	A	70	GLU	2.3
1	A	303	GLU	2.3
1	A	250	VAL	2.3
1	C	9	VAL	2.3
1	A	378	GLN	2.3
1	A	55	LYS	2.3
1	A	59	ILE	2.3
1	B	171	ILE	2.3
1	C	349	ILE	2.3
1	A	99	ALA	2.3
1	A	121	ALA	2.3
1	B	271	GLY	2.3
1	D	98	MET	2.3
1	A	66	ASN	2.3
1	B	77	VAL	2.3
1	D	293	ARG	2.3
1	A	180	PHE	2.3
1	C	157	PHE	2.3
1	D	226	PHE	2.3
1	A	16	ILE	2.3
1	A	268	THR	2.3
1	A	371	ILE	2.3
1	B	257	ILE	2.3
1	C	16	ILE	2.3
1	D	97	THR	2.3
1	A	311	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	216	MET	2.3
1	C	27	ASN	2.2
1	A	366	GLU	2.2
1	C	28	LEU	2.2
1	D	10	LEU	2.2
1	D	107	LEU	2.2
1	D	248	SER	2.2
1	A	82	GLY	2.2
1	B	8	THR	2.2
1	A	186	ALA	2.2
1	B	321	ARG	2.2
1	C	66	ASN	2.2
1	C	363	SER	2.2
1	D	69	LYS	2.2
1	C	384	GLU	2.2
1	B	166	ASP	2.2
1	B	236	PHE	2.2
1	A	85	ALA	2.2
1	A	100	ALA	2.2
1	D	90	ALA	2.2
1	D	138	ALA	2.2
1	C	114	ILE	2.2
1	D	76	SER	2.2
1	C	4	PRO	2.2
1	D	36	LEU	2.2
1	C	42	VAL	2.2
1	A	323	ALA	2.2
1	B	89	ALA	2.2
1	B	259	ALA	2.2
1	C	141	GLU	2.2
1	D	16	ILE	2.2
1	A	108	LYS	2.2
1	C	44	ASP	2.2
1	C	110	THR	2.2
1	C	98	MET	2.2
1	A	263	SER	2.2
1	C	63	SER	2.2
1	D	63	SER	2.2
1	D	360	ALA	2.2
1	C	269	PRO	2.2
1	B	66	ASN	2.2
1	A	47	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	241	HIS	2.2
1	A	134	LEU	2.2
1	B	146	LEU	2.2
1	B	274	LEU	2.2
1	C	144	THR	2.2
1	C	185	LEU	2.2
1	A	333	VAL	2.2
1	A	113	ALA	2.1
1	D	35	ALA	2.1
1	D	113	ALA	2.1
1	C	3	GLN	2.1
1	C	331	ILE	2.1
1	C	167	TYR	2.1
1	C	282	THR	2.1
1	D	111	LEU	2.1
1	D	234	GLU	2.1
1	D	41	ASN	2.1
1	A	94	ALA	2.1
1	A	109	ALA	2.1
1	B	178	GLY	2.1
1	B	360	ALA	2.1
1	D	162	HIS	2.1
1	B	144	THR	2.1
1	C	127	SER	2.1
1	C	377	ILE	2.1
1	D	363	SER	2.1
1	B	21	LEU	2.1
1	D	147	LEU	2.1
1	D	117	GLY	2.1
1	B	240	VAL	2.1
1	C	70	GLU	2.1
1	D	317	SER	2.1
1	A	231	ILE	2.1
1	A	266	MET	2.1
1	A	340	LYS	2.1
1	B	59	ILE	2.1
1	B	352	LYS	2.1
1	C	106	GLY	2.1
1	D	246	ILE	2.1
1	B	162	HIS	2.1
1	D	31	TYR	2.1
1	A	320	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	206	ALA	2.1
1	D	284	ALA	2.1
1	A	166	ASP	2.1
1	A	43	LYS	2.1
1	D	151	SER	2.1
1	B	359	PRO	2.1
1	B	261	ILE	2.1
1	B	276	TRP	2.1
1	A	326	ASN	2.1
1	B	147	LEU	2.1
1	B	292	LEU	2.1
1	A	363	SER	2.1
1	D	268	THR	2.1
1	B	148	PRO	2.1
1	A	343	PHE	2.0
1	B	34	ILE	2.0
1	C	226	PHE	2.0
1	A	147	LEU	2.0
1	B	151	SER	2.0
1	C	36	LEU	2.0
1	C	317	SER	2.0
1	B	350	VAL	2.0
1	B	153	HIS	2.0
1	A	278	LYS	2.0
1	A	313	GLU	2.0
1	A	345	ASP	2.0
1	A	123	ALA	2.0
1	C	80	ALA	2.0
1	D	123	ALA	2.0
1	A	246	ILE	2.0
1	A	289	PHE	2.0
1	D	32	GLN	2.0
1	D	96	TRP	2.0
1	C	129	VAL	2.0
1	C	277	PRO	2.0
1	C	249	MET	2.0
1	D	280	MET	2.0
1	A	19	SER	2.0
1	D	49	ALA	2.0
1	C	59	ILE	2.0
1	D	59	ILE	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, 95^{th} 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	ACT	C	1303	4/4	0.75	0.27	2.76	34,35,36,36	0
2	ACT	D	1304	4/4	0.63	0.26	1.75	29,32,33,34	0
2	ACT	B	1302	4/4	0.82	0.18	1.04	44,45,45,46	0
2	ACT	A	1301	4/4	0.62	0.27	0.84	29,30,30,31	0

6.5 Other polymers (i)

There are no such residues in this entry.