Full wwPDB X-ray Structure Validation Report (i)

Jun 13, 2024 – 08:39 AM EDT

PDB ID	:	4GRS
Title	:	Crystal structure of a chimeric DAH7PS
Authors	:	Cross, P.J.; Allison, T.M.; Dobson, R.C.J.; Jameson, G.B.; Parker, E.J.
Deposited on	:	2012-08-26
Resolution	:	3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

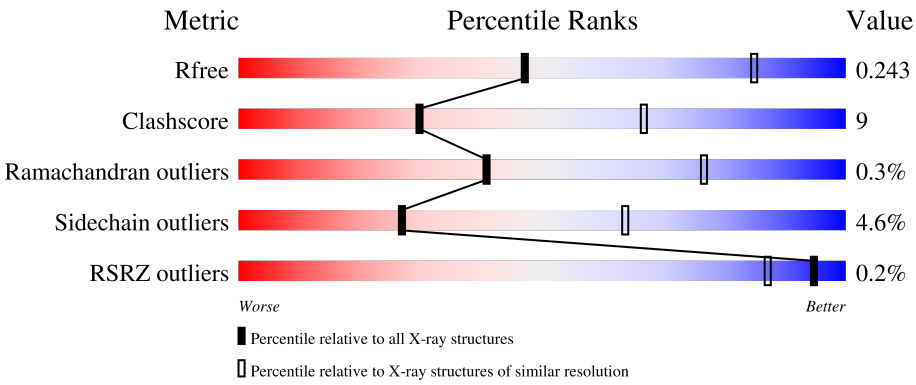
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	333	% 81% 18% •
1	B	333	83% 15% •
1	C	333	81% 16% •
1	D	333	80% 17% ••

2 Entry composition (i)

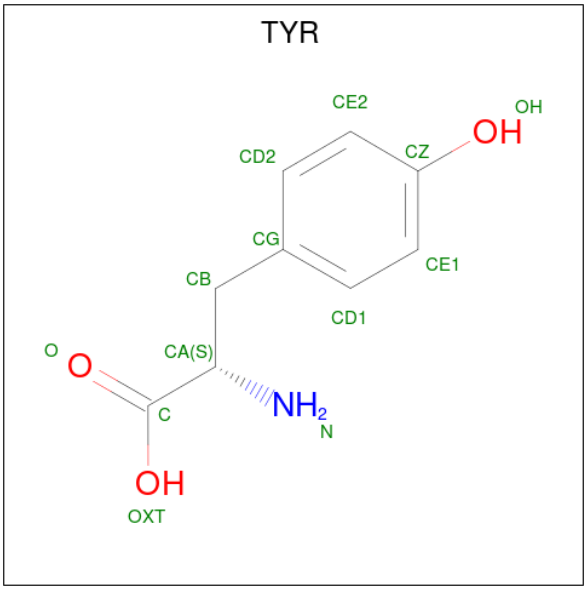
There are 3 unique types of molecules in this entry. The entry contains 10092 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Phospho-2-dehydro-3-deoxyheptonate aldolase, 2-dehydro-3-deoxyphosphoheptonate aldolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	333	2533	1614	427	481	11	0	0	0
1	B	333	2510	1600	422	477	11	0	0	0
1	C	332	2474	1575	413	475	11	0	0	0
1	D	331	2502	1595	419	477	11	0	0	0

- Molecule 2 is TYROSINE (three-letter code: TYR) (formula: $C_9H_{11}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	13	9	1	3	0	0
2	A	1	13	9	1	3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	B	1	13	9	1	3	0	0
			Total	C	N	O		
2	D	1	13	9	1	3	0	0

- Molecule 3 is water.

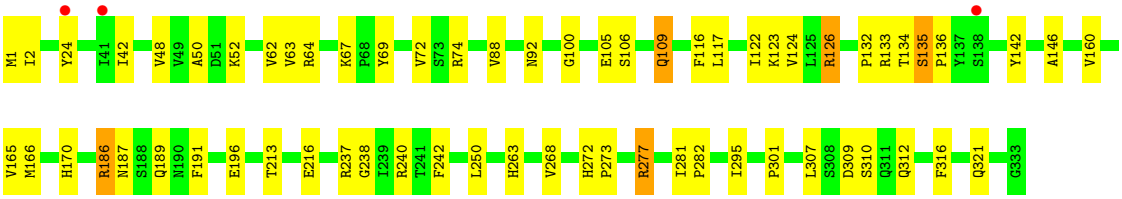
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	6	6	6	0	0
			Total	O		
3	B	7	7	7	0	0
			Total	O		
3	C	6	6	6	0	0
			Total	O		
3	D	2	2	2	0	0

3 Residue-property plots (i)

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

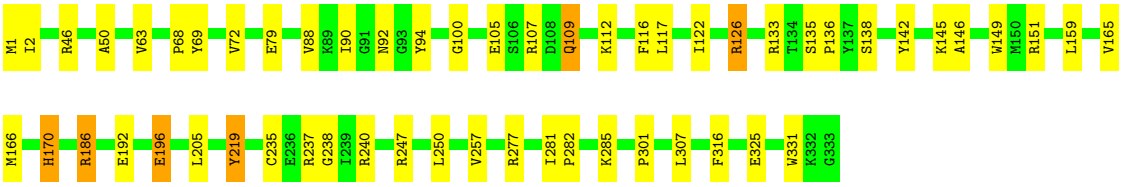
• Molecule 1: Phospho-2-dehydro-3-deoxyheptonate aldolase, 2-dehydro-3-deoxyphosphoheptona te aldolase

Chain A:



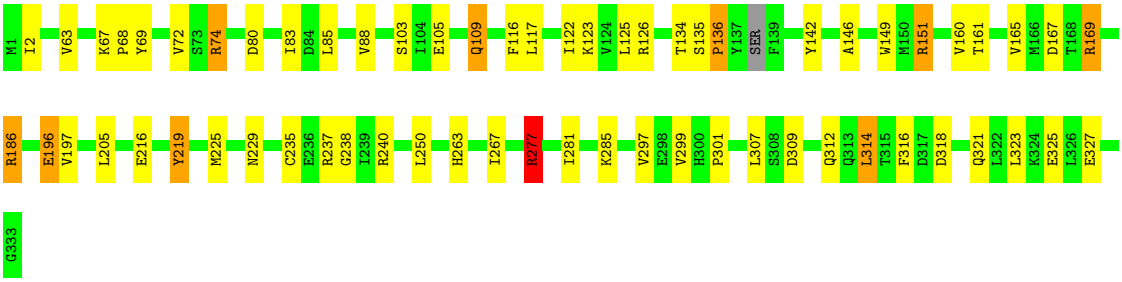
• Molecule 1: Phospho-2-dehydro-3-deoxyheptonate aldolase, 2-dehydro-3-deoxyphosphoheptona te aldolase

Chain B:



• Molecule 1: Phospho-2-dehydro-3-deoxyheptonate aldolase, 2-dehydro-3-deoxyphosphoheptona te aldolase

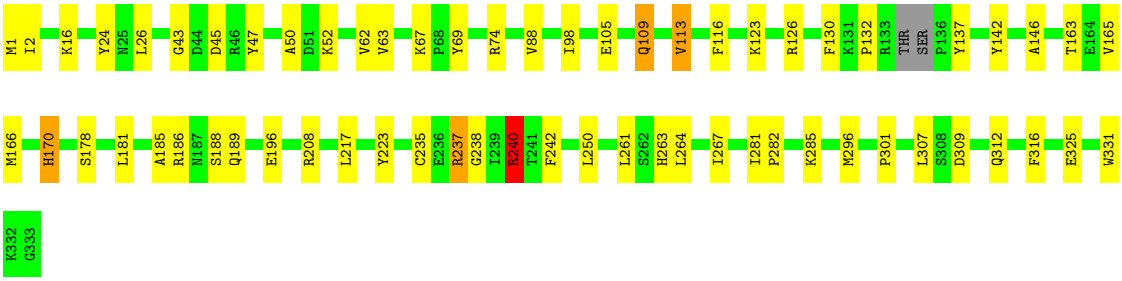
Chain C:



• Molecule 1: Phospho-2-dehydro-3-deoxyheptonate aldolase, 2-dehydro-3-deoxyphosphoheptona te aldolase

Chain D:

80%
17%


M1 I2 K16 Y24 N25 L26 G43 D44 D45 R46 Y47 A50 D51 K52 V62 V63 K67 P68 Y69 R74 V88 I98 E105 Q109 V113 F116 K123 R126 F130 K131 P132 R133 THR SER P136 Y137 Y142 A146 T163 E164 V165
M166 H170 S178 L181 A185 R186 N187 S188 Q189 E196 R208 L217 Y223 C235 E236 R237 G238 I239 R240 T241 F242 L250 L261 S262 H263 L264 I267 I281 P282 K285 M296 P301 L307 S308 D309 Q312 F316 E325 W331
K332 G333

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	76.90Å 130.85Å 138.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.94 – 3.00 37.94 – 3.00	Depositor EDS
% Data completeness (in resolution range)	94.5 (37.94-3.00) 94.6 (37.94-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	3.81 (at 3.01Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.192 , 0.248 0.189 , 0.243	Depositor DCC
R_{free} test set	1350 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	67.5	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 57.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10092	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 4.18% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	0.43	0/2576	0.60	1/3497 (0.0%)
1	B	0.43	2/2552 (0.1%)	0.61	4/3467 (0.1%)
1	C	0.44	1/2514 (0.0%)	0.65	6/3422 (0.2%)
1	D	0.45	1/2544 (0.0%)	0.62	2/3455 (0.1%)
All	All	0.44	4/10186 (0.0%)	0.62	13/13841 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	149	TRP	CD2-CE2	5.53	1.48	1.41
1	B	331	TRP	CD2-CE2	5.10	1.47	1.41
1	C	149	TRP	CD2-CE2	5.04	1.47	1.41
1	D	331	TRP	CD2-CE2	5.02	1.47	1.41

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	277	ARG	NE-CZ-NH2	7.59	124.09	120.30
1	B	257	VAL	CG1-CB-CG2	-6.99	99.72	110.90
1	C	74	ARG	NE-CZ-NH1	-6.98	116.81	120.30
1	A	277	ARG	NE-CZ-NH1	6.79	123.69	120.30
1	C	74	ARG	NE-CZ-NH2	6.32	123.46	120.30
1	C	297	VAL	CG1-CB-CG2	-6.17	101.02	110.90
1	B	107	ARG	NE-CZ-NH2	5.93	123.27	120.30
1	D	113	VAL	CG1-CB-CG2	-5.91	101.44	110.90
1	D	240	ARG	NE-CZ-NH1	-5.71	117.44	120.30
1	B	277	ARG	NE-CZ-NH2	5.63	123.12	120.30
1	C	169	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	C	197	VAL	CG1-CB-CG2	-5.08	102.77	110.90
1	B	107	ARG	NE-CZ-NH1	-5.03	117.78	120.30

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	2533	0	2519	62	0
1	B	2510	0	2484	39	0
1	C	2474	0	2402	48	0
1	D	2502	0	2462	59	0
2	A	26	0	16	1	0
2	B	13	0	8	0	0
2	D	13	0	8	0	0
3	A	6	0	0	2	0
3	B	7	0	0	0	0
3	C	6	0	0	0	0
3	D	2	0	0	0	0
All	All	10092	0	9899	188	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 9.

All (188) 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:D:166:MET:CE	1:D:186:ARG:HH21	1.76	0.97
1:C:196:GLU:HA	1:C:196:GLU:OE1	1.69	0.93
1:A:186:ARG:NH2	1:D:189:GLN:O	2.02	0.93
1:A:134:THR:O	1:D:223:TYR:CD1	2.22	0.92
1:B:105:GLU:H	1:B:109:GLN:HE21	1.19	0.91
1:A:135:SER:H	1:A:136:PRO:CD	1.84	0.90
1:C:277:ARG:HB2	1:C:277:ARG:HH21	1.39	0.88
1:D:166:MET:HE3	1:D:186:ARG:HH21	1.44	0.82
1:A:135:SER:H	1:A:136:PRO:HD3	1.45	0.80
1:D:105:GLU:H	1:D:109:GLN:HE21	1.30	0.79
1:B:301:PRO:HA	1:B:316:PHE:CE1	2.18	0.78
1:A:105:GLU:H	1:A:109:GLN:HE21	1.29	0.77
1:D:24:TYR:OH	1:D:52:LYS:HG3	1.86	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:ARG:CB	1:B:138:SER:HB2	2.17	0.74
1:A:135:SER:N	1:A:136:PRO:CD	2.49	0.73
1:A:301:PRO:HA	1:A:316:PHE:CE1	2.23	0.72
1:C:105:GLU:H	1:C:109:GLN:HE21	1.39	0.70
1:D:166:MET:HE2	1:D:186:ARG:HH21	1.55	0.70
1:B:301:PRO:CA	1:B:316:PHE:HE1	2.05	0.70
1:D:301:PRO:HA	1:D:316:PHE:CE1	2.27	0.69
1:A:189:GLN:O	1:D:186:ARG:NH1	2.26	0.69
1:B:196:GLU:HA	1:B:196:GLU:OE1	1.92	0.68
1:B:196:GLU:OE2	1:C:169:ARG:NH2	2.28	0.67
1:B:105:GLU:N	1:B:109:GLN:HE21	1.91	0.66
1:C:74:ARG:NH2	1:C:263:HIS:HA	2.14	0.63
1:B:196:GLU:CD	1:C:169:ARG:HH22	2.03	0.62
1:A:191:PHE:H	1:D:186:ARG:HH12	1.47	0.62
1:A:281:ILE:HD12	1:A:281:ILE:H	1.65	0.60
1:B:69:TYR:HB2	1:B:72:VAL:HG22	1.83	0.60
1:D:281:ILE:HB	1:D:282:PRO:HD3	1.82	0.59
1:A:136:PRO:HB3	1:D:47:TYR:CD1	2.37	0.59
1:C:301:PRO:HA	1:C:316:PHE:CE1	2.37	0.59
1:C:88:VAL:CG2	1:C:123:LYS:CB	2.81	0.59
1:D:109:GLN:O	1:D:113:VAL:HG23	2.03	0.58
1:A:2:ILE:HD13	1:C:2:ILE:HD13	1.84	0.58
1:A:105:GLU:HB2	1:A:109:GLN:HG3	1.85	0.58
1:A:48:VAL:O	1:A:64:ARG:NH2	2.36	0.57
1:C:88:VAL:CG2	1:C:123:LYS:HB3	2.35	0.57
1:D:88:VAL:CG2	1:D:123:LYS:HB2	2.34	0.57
1:A:24:TYR:OH	1:A:52:LYS:HG3	2.05	0.56
1:A:301:PRO:CA	1:A:316:PHE:HE1	2.19	0.56
1:B:301:PRO:HA	1:B:316:PHE:CD1	2.40	0.56
1:D:105:GLU:N	1:D:109:GLN:HE21	2.03	0.55
1:C:85:LEU:HD23	1:C:160:VAL:HG21	1.88	0.55
1:D:88:VAL:CG2	1:D:123:LYS:CB	2.84	0.55
1:A:88:VAL:CG2	1:A:123:LYS:CB	2.85	0.55
1:C:323:LEU:O	1:C:327:GLU:HG2	2.07	0.54
1:D:301:PRO:CA	1:D:316:PHE:HE1	2.19	0.54
1:A:105:GLU:N	1:A:109:GLN:HE21	2.03	0.54
1:A:186:ARG:NH2	1:A:186:ARG:HG3	2.23	0.54
1:A:1:MET:HE1	1:A:50:ALA:HA	1.89	0.54
1:A:135:SER:H	1:A:136:PRO:HD2	1.71	0.53
1:B:301:PRO:CA	1:B:316:PHE:CE1	2.84	0.53
1:A:135:SER:N	1:A:136:PRO:HD2	2.22	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:301:PRO:CA	1:D:316:PHE:CE1	2.92	0.53
1:B:238:GLY:HA2	1:B:250:LEU:HA	1.91	0.53
1:C:69:TYR:HB2	1:C:72:VAL:HG22	1.91	0.52
1:D:301:PRO:HA	1:D:316:PHE:CD1	2.44	0.52
1:C:238:GLY:HA2	1:C:250:LEU:HA	1.91	0.52
1:A:106:SER:OG	1:A:109:GLN:HB2	2.09	0.52
1:A:134:THR:O	1:D:223:TYR:CE1	2.61	0.52
1:B:281:ILE:H	1:B:281:ILE:HD12	1.74	0.52
1:D:166:MET:CE	1:D:186:ARG:NH2	2.59	0.52
1:D:116:PHE:HB2	1:D:316:PHE:HE2	1.76	0.51
1:A:166:MET:H	1:A:170:HIS:HE1	1.57	0.51
1:D:166:MET:HE2	1:D:186:ARG:NH2	2.22	0.51
1:A:105:GLU:H	1:A:109:GLN:NE2	2.04	0.51
1:A:186:ARG:HG3	1:A:186:ARG:HH21	1.76	0.51
1:A:88:VAL:CG2	1:A:123:LYS:HB3	2.42	0.50
1:A:67:LYS:HD3	1:A:69:TYR:OH	2.12	0.50
1:A:126:ARG:NH2	3:A:501:HOH:O	2.45	0.50
1:C:281:ILE:H	1:C:281:ILE:HD12	1.77	0.50
1:B:63:VAL:HG21	1:D:63:VAL:HG11	1.92	0.50
1:C:88:VAL:CG2	1:C:123:LYS:HB2	2.42	0.50
1:D:196:GLU:HA	1:D:196:GLU:OE1	2.10	0.50
1:B:281:ILE:HB	1:B:282:PRO:HD3	1.94	0.50
1:B:135:SER:HB2	1:B:136:PRO:HD2	1.93	0.49
1:A:133:ARG:CB	1:A:136:PRO:HG2	2.43	0.49
1:D:1:MET:CE	1:D:62:VAL:HG11	2.42	0.49
1:A:88:VAL:CG2	1:A:123:LYS:HB2	2.43	0.49
1:D:69:TYR:OH	1:D:261:LEU:HD12	2.12	0.49
1:B:2:ILE:HD13	1:D:2:ILE:HD13	1.94	0.49
1:C:105:GLU:N	1:C:109:GLN:HE21	2.06	0.49
1:A:63:VAL:HG11	1:C:63:VAL:HG21	1.95	0.49
1:C:74:ARG:NH1	1:C:80:ASP:OD1	2.42	0.49
1:D:142:TYR:HB2	1:D:146:ALA:HB2	1.93	0.49
1:D:1:MET:HE1	1:D:50:ALA:HA	1.93	0.49
1:A:242:PHE:CG	1:C:240:ARG:HG2	2.48	0.48
1:A:301:PRO:HA	1:A:316:PHE:CD1	2.48	0.48
1:B:117:LEU:HB3	1:B:122:ILE:HB	1.95	0.48
1:D:238:GLY:HA2	1:D:250:LEU:HA	1.95	0.48
1:C:277:ARG:HH21	1:C:277:ARG:CB	2.19	0.47
1:A:117:LEU:HB3	1:A:122:ILE:HB	1.96	0.47
1:A:166:MET:CE	1:A:186:ARG:HH11	2.27	0.47
1:A:196:GLU:OE1	1:A:196:GLU:HA	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:ARG:NH2	1:A:310:SER:O	2.48	0.47
1:B:240:ARG:HG2	1:D:242:PHE:CB	2.45	0.47
1:C:116:PHE:CG	1:C:316:PHE:CD2	3.02	0.47
1:D:1:MET:HE3	1:D:62:VAL:HG11	1.96	0.47
1:D:26:LEU:HD22	1:D:43:GLY:HA3	1.96	0.47
1:A:301:PRO:CA	1:A:316:PHE:CE1	2.92	0.46
1:C:105:GLU:HB2	1:C:109:GLN:HG2	1.97	0.46
1:C:117:LEU:HB3	1:C:122:ILE:HB	1.96	0.46
1:D:1:MET:HB2	1:D:45:ASP:OD2	2.15	0.46
1:A:74:ARG:NH2	1:A:263:HIS:HA	2.31	0.46
1:C:196:GLU:OE1	1:C:196:GLU:CA	2.53	0.46
1:A:1:MET:CE	1:A:62:VAL:HG11	2.46	0.46
1:A:142:TYR:HB2	1:A:146:ALA:HB2	1.98	0.46
1:C:235:CYS:HA	1:C:267:ILE:O	2.15	0.46
1:A:69:TYR:HB2	1:A:72:VAL:HG22	1.97	0.46
1:B:205:LEU:HD11	1:B:235:CYS:HB2	1.96	0.46
1:A:1:MET:HE3	1:A:62:VAL:HG11	1.98	0.46
1:A:216:GLU:OE1	1:D:240:ARG:NH1	2.49	0.46
1:C:314:LEU:HG	1:C:318:ASP:HB3	1.97	0.46
1:D:67:LYS:HD3	1:D:69:TYR:OH	2.15	0.46
1:A:242:PHE:CB	1:C:240:ARG:HG2	2.45	0.45
1:A:124:VAL:HG13	1:A:160:VAL:HG23	1.98	0.45
1:B:240:ARG:HG2	1:D:242:PHE:CG	2.51	0.45
1:B:116:PHE:CG	1:B:316:PHE:CD2	3.04	0.45
1:C:88:VAL:HG22	1:C:123:LYS:CB	2.46	0.45
1:C:186:ARG:H	1:C:186:ARG:HG2	1.57	0.45
1:D:88:VAL:HG22	1:D:123:LYS:HB2	1.98	0.45
1:A:100:GLY:HA3	1:A:126:ARG:HG3	1.98	0.44
1:A:238:GLY:HA2	1:A:250:LEU:HA	1.99	0.44
1:C:301:PRO:CA	1:C:316:PHE:CE1	3.00	0.44
1:C:125:LEU:O	1:C:161:THR:HA	2.17	0.44
1:D:309:ASP:HB3	1:D:312:GLN:HG2	1.99	0.44
1:B:166:MET:H	1:B:170:HIS:HE1	1.64	0.44
1:C:285:LYS:HD3	1:C:325:GLU:HB3	1.99	0.44
1:A:42:ILE:HA	2:A:401:TYR:O	2.18	0.44
1:A:166:MET:H	1:A:170:HIS:CE1	2.35	0.44
1:B:151:ARG:HE	1:B:151:ARG:HA	1.83	0.44
1:D:16:LYS:HA	1:D:16:LYS:HD2	1.89	0.44
1:D:166:MET:H	1:D:170:HIS:HE1	1.66	0.44
1:B:68:PRO:CB	1:B:219:TYR:OH	2.66	0.43
1:D:88:VAL:HG21	1:D:123:LYS:HB2	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:TYR:HB2	1:B:146:ALA:HB2	2.00	0.43
1:C:116:PHE:HB2	1:C:316:PHE:HE2	1.83	0.43
1:C:309:ASP:HB3	1:C:312:GLN:HG2	1.99	0.43
1:B:285:LYS:HD3	1:B:325:GLU:HB3	2.01	0.43
1:C:68:PRO:HB2	1:C:219:TYR:CE1	2.54	0.43
1:B:116:PHE:HB2	1:B:316:PHE:HE2	1.83	0.43
1:D:185:ALA:O	1:D:188:SER:HB2	2.19	0.43
1:C:142:TYR:HB2	1:C:146:ALA:HB2	2.01	0.43
1:D:116:PHE:CG	1:D:316:PHE:CD2	3.05	0.43
1:D:163:THR:HG22	1:D:178:SER:CB	2.48	0.43
1:D:237:ARG:C	1:D:237:ARG:HD3	2.39	0.43
1:C:205:LEU:HD11	1:C:235:CYS:HB2	1.99	0.43
1:A:281:ILE:HD12	1:A:281:ILE:N	2.32	0.43
1:A:116:PHE:HB2	1:A:316:PHE:HE2	1.83	0.42
1:A:268:VAL:O	1:A:295:ILE:HA	2.18	0.42
1:C:67:LYS:HD3	1:C:69:TYR:OH	2.19	0.42
1:C:83:ILE:HG22	1:C:85:LEU:CD1	2.49	0.42
1:D:285:LYS:HD3	1:D:325:GLU:HB3	1.99	0.42
1:B:105:GLU:HB2	1:B:109:GLN:HG2	2.00	0.42
1:C:225:MET:HA	1:C:229:ASN:O	2.19	0.42
1:B:63:VAL:HG11	1:D:63:VAL:HG21	2.00	0.42
1:B:112:LYS:HB2	1:B:112:LYS:HE3	1.92	0.42
1:A:116:PHE:CG	1:A:316:PHE:CD2	3.08	0.42
1:C:167:ASP:OD1	1:C:169:ARG:HD2	2.19	0.42
1:C:151:ARG:HA	1:C:151:ARG:HD3	1.43	0.42
1:A:1:MET:CE	1:A:50:ALA:HA	2.50	0.42
1:A:281:ILE:HB	1:A:282:PRO:HD3	2.01	0.42
1:D:88:VAL:CG2	1:D:123:LYS:HB3	2.50	0.42
1:B:116:PHE:CB	1:B:316:PHE:HE2	2.33	0.42
1:B:186:ARG:H	1:B:186:ARG:HG2	1.56	0.41
1:D:98:ILE:O	1:D:296:MET:HA	2.19	0.41
1:B:192:GLU:HG2	1:C:167:ASP:HB2	2.02	0.41
1:A:309:ASP:HB3	1:A:312:GLN:HG2	2.03	0.41
1:B:1:MET:CE	1:B:50:ALA:HA	2.50	0.41
1:D:208:ARG:HB2	1:D:217:LEU:HD13	2.01	0.41
1:C:88:VAL:HG22	1:C:123:LYS:HB2	2.02	0.41
1:D:105:GLU:HB2	1:D:109:GLN:HG2	2.03	0.41
1:D:1:MET:CE	1:D:50:ALA:HA	2.50	0.41
1:B:79:GLU:H	1:B:79:GLU:CD	2.24	0.41
1:C:116:PHE:CB	1:C:316:PHE:CE2	3.04	0.41
1:D:116:PHE:CB	1:D:316:PHE:CE2	3.04	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:THR:HB	3:A:504:HOH:O	2.20	0.41
1:B:92:ASN:C	1:B:94:TYR:H	2.23	0.41
1:D:130:PHE:CD1	1:D:130:PHE:N	2.88	0.41
1:D:264:LEU:HD23	1:D:264:LEU:HA	1.94	0.41
1:B:240:ARG:HH12	1:C:216:GLU:CD	2.25	0.41
1:D:74:ARG:NH2	1:D:263:HIS:HA	2.35	0.40
1:D:235:CYS:HA	1:D:267:ILE:O	2.21	0.40
1:A:186:ARG:HG2	1:A:187:ASN:N	2.36	0.40
1:C:135:SER:HA	1:C:136:PRO:HD2	1.77	0.40
1:A:272:HIS:N	1:A:273:PRO:HD2	2.36	0.40
1:B:100:GLY:HA3	1:B:126:ARG:O	2.22	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	331/333 (99%)	316 (96%)	13 (4%)	2 (1%)	25	64
1	B	331/333 (99%)	317 (96%)	14 (4%)	0	100	100
1	C	328/333 (98%)	313 (95%)	14 (4%)	1 (0%)	41	76
1	D	327/333 (98%)	311 (95%)	15 (5%)	1 (0%)	41	76
All	All	1317/1332 (99%)	1257 (95%)	56 (4%)	4 (0%)	41	76

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	132	PRO
1	A	132	PRO
1	A	135	SER
1	C	136	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	267/285 (94%)	258 (97%)	9 (3%)	37	72
1	B	262/285 (92%)	247 (94%)	15 (6%)	20	56
1	C	253/285 (89%)	238 (94%)	15 (6%)	19	54
1	D	261/285 (92%)	252 (97%)	9 (3%)	37	72
All	All	1043/1140 (92%)	995 (95%)	48 (5%)	27	64

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	ASN
1	A	109	GLN
1	A	126	ARG
1	A	165	VAL
1	A	186	ARG
1	A	237	ARG
1	A	240	ARG
1	A	307	LEU
1	A	321	GLN
1	B	46	ARG
1	B	88	VAL
1	B	90	ILE
1	B	109	GLN
1	B	126	ARG
1	B	145	LYS
1	B	159	LEU
1	B	165	VAL
1	B	170	HIS
1	B	186	ARG
1	B	196	GLU
1	B	219	TYR
1	B	237	ARG
1	B	247	ARG
1	B	307	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	103	SER
1	C	109	GLN
1	C	126	ARG
1	C	134	THR
1	C	151	ARG
1	C	165	VAL
1	C	186	ARG
1	C	196	GLU
1	C	219	TYR
1	C	237	ARG
1	C	277	ARG
1	C	299	VAL
1	C	307	LEU
1	C	314	LEU
1	C	321	GLN
1	D	109	GLN
1	D	126	ARG
1	D	137	TYR
1	D	165	VAL
1	D	170	HIS
1	D	181	LEU
1	D	237	ARG
1	D	240	ARG
1	D	307	LEU

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

Mol	Chain	Res	Type
1	A	92	ASN
1	A	109	GLN
1	A	170	HIS
1	A	321	GLN
1	B	109	GLN
1	B	212	ASN
1	C	109	GLN
1	C	212	ASN
1	C	321	GLN
1	D	109	GLN
1	D	170	HIS
1	D	212	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	TYR	B	401	-	12,13,13	0.68	0	13,17,17	0.77	1 (7%)
2	TYR	D	401	-	12,13,13	0.78	1 (8%)	13,17,17	0.73	1 (7%)
2	TYR	A	402	-	12,13,13	0.72	1 (8%)	13,17,17	0.83	1 (7%)
2	TYR	A	401	-	12,13,13	0.77	1 (8%)	13,17,17	0.81	1 (7%)

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	TYR	B	401	-	-	0/8/8/8	0/1/1/1
2	TYR	D	401	-	-	1/8/8/8	0/1/1/1
2	TYR	A	402	-	-	1/8/8/8	0/1/1/1
2	TYR	A	401	-	-	2/8/8/8	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	TYR	OXT-C	-2.20	1.23	1.30
2	A	402	TYR	OXT-C	-2.15	1.23	1.30
2	A	401	TYR	OXT-C	-2.00	1.24	1.30

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	402	TYR	OXT-C-O	-2.86	117.58	124.08
2	A	401	TYR	OXT-C-O	-2.77	117.80	124.08
2	B	401	TYR	OXT-C-O	-2.54	118.31	124.08
2	D	401	TYR	OXT-C-O	-2.54	118.31	124.08

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	TYR	OXT-C-CA-N
2	A	402	TYR	OXT-C-CA-N
2	A	401	TYR	O-C-CA-N
2	D	401	TYR	O-C-CA-N

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	TYR	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	333/333 (100%)	-0.43	3 (0%)	84	63	37, 75, 126, 167	0
1	B	333/333 (100%)	-0.35	0	100	100	39, 80, 127, 165	0
1	C	332/333 (99%)	-0.33	0	100	100	35, 79, 173, 221	0
1	D	331/333 (99%)	-0.52	0	100	100	33, 76, 115, 166	0
All	All	1329/1332 (99%)	-0.41	3 (0%)	95	87	33, 77, 139, 221	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	138	SER	2.9
1	A	41	ILE	2.5
1	A	24	TYR	2.4

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	TYR	A	401	13/13	0.95	0.36	57,66,74,76	0
2	TYR	A	402	13/13	0.95	0.43	68,70,86,89	0
2	TYR	D	401	13/13	0.96	0.35	45,61,70,73	0
2	TYR	B	401	13/13	0.97	0.29	52,59,69,69	0

6.5 Other polymers (i)

There are no such residues in this entry.