



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:06 AM GMT

PDB ID : 3H6K
Title : Crystal Structure of Human 11-beta-hydroxysteroid-dehydrogenase Bound to an Ortho-chloro-sulfonyl-piperazine Inhibitor
Authors : Bard, J.; Svenson, K.
Deposited on : 2009-04-23
Resolution : 2.19 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

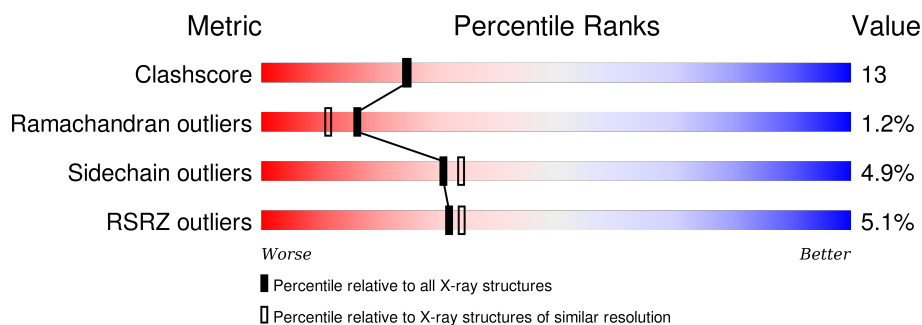
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.19 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))
Clashscore	102246	5965 (2.20-2.16)
Ramachandran outliers	100387	5863 (2.20-2.16)
Sidechain outliers	100360	5864 (2.20-2.16)
RSRZ outliers	91569	5142 (2.20-2.16)

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	286	<div> <div>3%</div> <div> <div></div> <div>63%</div> <div>25%</div> <div>•</div> <div>9%</div> </div> </div>
1	B	286	<div> <div>5%</div> <div> <div></div> <div>62%</div> <div>26%</div> <div>•</div> <div>9%</div> </div> </div>
1	C	286	<div> <div>5%</div> <div> <div></div> <div>70%</div> <div>19%</div> <div>•</div> <div>9%</div> </div> </div>
1	D	286	<div> <div>5%</div> <div> <div></div> <div>60%</div> <div>26%</div> <div>•</div> <div>10%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8306 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 Corticosteroid 11-beta-dehydrogenase isozyme 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	0	0
			1957	1246	334	363	14			
1	B	261	Total	C	N	O	S	1	1	0
			1984	1265	335	370	14			
1	C	260	Total	C	N	O	S	1	0	0
			1966	1252	335	364	15			
1	D	256	Total	C	N	O	S	3	0	0
			1934	1232	329	358	15			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	MET	-	EXPRESSION TAG	UNP P28845
A	8	LYS	-	EXPRESSION TAG	UNP P28845
A	9	HIS	-	EXPRESSION TAG	UNP P28845
A	10	GLN	-	EXPRESSION TAG	UNP P28845
A	11	HIS	-	EXPRESSION TAG	UNP P28845
A	12	GLN	-	EXPRESSION TAG	UNP P28845
A	13	HIS	-	EXPRESSION TAG	UNP P28845
A	14	GLN	-	EXPRESSION TAG	UNP P28845
A	15	HIS	-	EXPRESSION TAG	UNP P28845
A	16	GLN	-	EXPRESSION TAG	UNP P28845
A	17	HIS	-	EXPRESSION TAG	UNP P28845
A	18	GLN	-	EXPRESSION TAG	UNP P28845
A	19	HIS	-	EXPRESSION TAG	UNP P28845
A	20	GLN	-	EXPRESSION TAG	UNP P28845
A	21	GLN	-	EXPRESSION TAG	UNP P28845
A	22	PRO	-	EXPRESSION TAG	UNP P28845
A	23	LEU	-	EXPRESSION TAG	UNP P28845
A	272	SER	CYS	ENGINEERED	UNP P28845
B	7	MET	-	EXPRESSION TAG	UNP P28845
B	8	LYS	-	EXPRESSION TAG	UNP P28845
B	9	HIS	-	EXPRESSION TAG	UNP P28845

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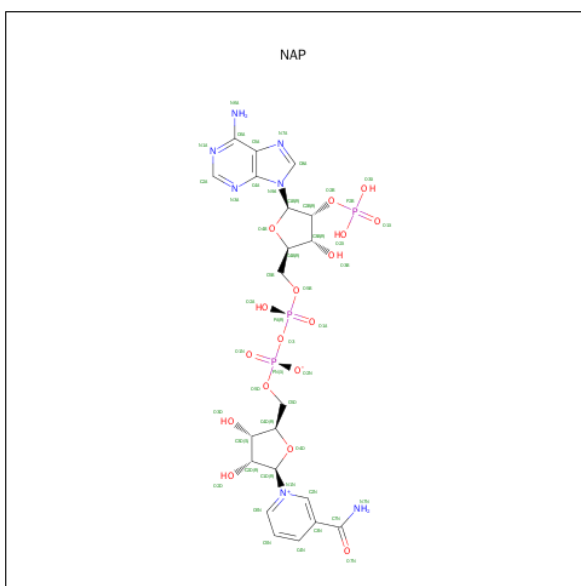
Chain	Residue	Modelled	Actual	Comment	Reference
B	10	GLN	-	EXPRESSION TAG	UNP P28845
B	11	HIS	-	EXPRESSION TAG	UNP P28845
B	12	GLN	-	EXPRESSION TAG	UNP P28845
B	13	HIS	-	EXPRESSION TAG	UNP P28845
B	14	GLN	-	EXPRESSION TAG	UNP P28845
B	15	HIS	-	EXPRESSION TAG	UNP P28845
B	16	GLN	-	EXPRESSION TAG	UNP P28845
B	17	HIS	-	EXPRESSION TAG	UNP P28845
B	18	GLN	-	EXPRESSION TAG	UNP P28845
B	19	HIS	-	EXPRESSION TAG	UNP P28845
B	20	GLN	-	EXPRESSION TAG	UNP P28845
B	21	GLN	-	EXPRESSION TAG	UNP P28845
B	22	PRO	-	EXPRESSION TAG	UNP P28845
B	23	LEU	-	EXPRESSION TAG	UNP P28845
B	272	SER	CYS	ENGINEERED	UNP P28845
C	7	MET	-	EXPRESSION TAG	UNP P28845
C	8	LYS	-	EXPRESSION TAG	UNP P28845
C	9	HIS	-	EXPRESSION TAG	UNP P28845
C	10	GLN	-	EXPRESSION TAG	UNP P28845
C	11	HIS	-	EXPRESSION TAG	UNP P28845
C	12	GLN	-	EXPRESSION TAG	UNP P28845
C	13	HIS	-	EXPRESSION TAG	UNP P28845
C	14	GLN	-	EXPRESSION TAG	UNP P28845
C	15	HIS	-	EXPRESSION TAG	UNP P28845
C	16	GLN	-	EXPRESSION TAG	UNP P28845
C	17	HIS	-	EXPRESSION TAG	UNP P28845
C	18	GLN	-	EXPRESSION TAG	UNP P28845
C	19	HIS	-	EXPRESSION TAG	UNP P28845
C	20	GLN	-	EXPRESSION TAG	UNP P28845
C	21	GLN	-	EXPRESSION TAG	UNP P28845
C	22	PRO	-	EXPRESSION TAG	UNP P28845
C	23	LEU	-	EXPRESSION TAG	UNP P28845
C	272	SER	CYS	ENGINEERED	UNP P28845
D	7	MET	-	EXPRESSION TAG	UNP P28845
D	8	LYS	-	EXPRESSION TAG	UNP P28845
D	9	HIS	-	EXPRESSION TAG	UNP P28845
D	10	GLN	-	EXPRESSION TAG	UNP P28845
D	11	HIS	-	EXPRESSION TAG	UNP P28845
D	12	GLN	-	EXPRESSION TAG	UNP P28845
D	13	HIS	-	EXPRESSION TAG	UNP P28845
D	14	GLN	-	EXPRESSION TAG	UNP P28845
D	15	HIS	-	EXPRESSION TAG	UNP P28845

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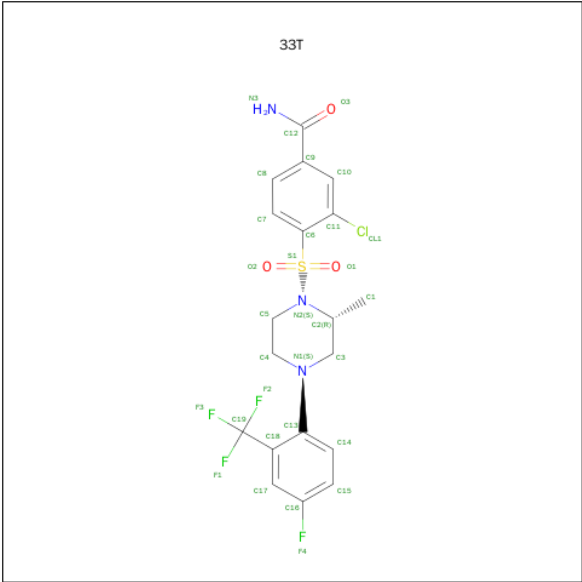
Chain	Residue	Modelled	Actual	Comment	Reference
D	16	GLN	-	EXPRESSION TAG	UNP P28845
D	17	HIS	-	EXPRESSION TAG	UNP P28845
D	18	GLN	-	EXPRESSION TAG	UNP P28845
D	19	HIS	-	EXPRESSION TAG	UNP P28845
D	20	GLN	-	EXPRESSION TAG	UNP P28845
D	21	GLN	-	EXPRESSION TAG	UNP P28845
D	22	PRO	-	EXPRESSION TAG	UNP P28845
D	23	LEU	-	EXPRESSION TAG	UNP P28845
D	272	SER	CYS	ENGINEERED	UNP P28845

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is 3-CHLORO-4-((2R)-4-[4-FLUORO-2-(TRIFLUOROMETHYL)PHENYL]-2-METHYLPIPERAZIN-1-YL}SULFONYL)BENZAMIDE (three-letter code: 33T) (formula: $C_{19}H_{18}ClF_4N_3O_3S$).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	A	1	Total	C	Cl	F	N	O	S	0	0
			31	19	1	4	3	3	1		
3	B	1	Total	C	Cl	F	N	O	S	0	0
			31	19	1	4	3	3	1		
3	C	1	Total	C	Cl	F	N	O	S	0	0
			31	19	1	4	3	3	1		
3	D	1	Total	C	Cl	F	N	O	S	0	0
			31	19	1	4	3	3	1		

- Molecule 4 is water.

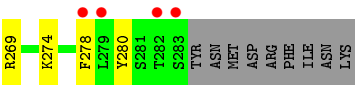
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	37	Total	O	0	0
			37	37		
4	B	32	Total	O	0	0
			32	32		
4	C	54	Total	O	0	0
			54	54		
4	D	26	Total	O	0	0
			26	26		

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.

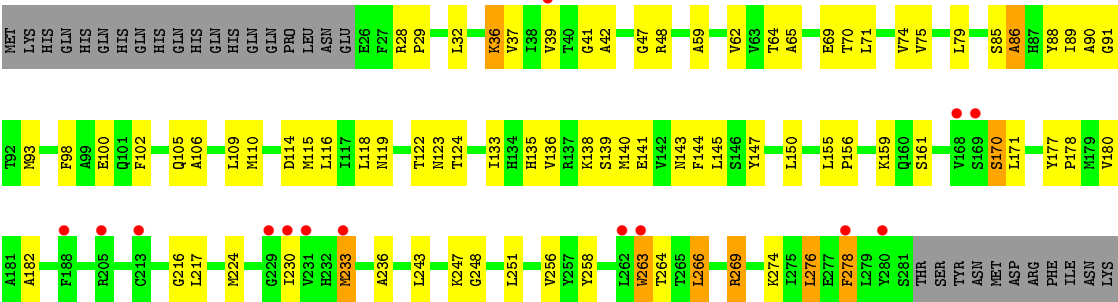
- Chain A:
-
- 3% 63% 25% 9%
- MET LYS GLN HIS GLN HIS GLN HIS GLN PRO ASN GLU E26 F27 R28 L32 K36 T40 G41 A42 S43 K44 G45 R48 E49 L54 A55 K56 V61 V62 V63 T64 K68 Q72 K73 V74 H77 C78 L81 M110 D114 E232 P237 K238 E239 E240 G248 V256 Y257 Y258 D259 S260 S261 L262 K263 T264 T265 L266 R269 S272 R273 K274 L275 L276 E277 F278 Y280 S283 Y284 K285 MET ASP ARG PHE ILE ASN LYS

- [illegible]

- Chain C:



● Molecule 1: Corticosteroid 11-beta-dehydrogenase isozyme 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	56.20Å 152.01Å 74.54Å 90.00° 92.41° 90.00°	Depositor
Resolution (Å)	31.47 – 2.19 31.47 – 2.19	Depositor EDS
% Data completeness (in resolution range)	66.2 (31.47-2.19) 66.2 (31.47-2.19)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 2.18Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.190 , 0.275 0.196 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	31.2	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 53.9	EDS
Estimated twinning fraction	0.059 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 51679 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8306	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% 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: 33T, NAP

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	0.32	0/1988	0.53	0/2685
1	B	0.32	0/2019	0.51	0/2726
1	C	0.33	0/1997	0.52	0/2697
1	D	0.30	0/1965	0.52	0/2652
All	All	0.32	0/7969	0.52	0/10760

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	1957	0	1976	56	0
1	B	1984	0	2019	59	0
1	C	1966	0	2005	45	0
1	D	1934	0	1965	65	0
2	A	48	0	25	3	0
2	B	48	0	25	6	0
2	C	48	0	25	5	0
2	D	48	0	25	5	0
3	A	31	0	18	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	31	0	18	3	0
3	C	31	0	18	1	0
3	D	31	0	18	2	0
4	A	37	0	0	0	0
4	B	32	0	0	0	0
4	C	54	0	0	2	0
4	D	26	0	0	3	0
All	All	8306	0	8137	209	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 13.

All (209) 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:269:ARG:NH2	1:B:274:LYS:HE2	1.80	0.96
1:D:170:SER:HB3	2:D:1:NAP:H5N	1.61	0.81
1:D:71:LEU:HD13	1:D:88:TYR:HB2	1.67	0.77
1:A:283:SER:N	1:A:284:TYR:HA	1.99	0.76
1:B:64:THR:HB	1:B:102:PHE:CE1	2.23	0.73
1:B:170:SER:OG	2:B:1:NAP:H6N	1.88	0.73
1:C:170:SER:HB3	2:C:1:NAP:H5N	1.71	0.73
1:A:221:GLU:H	1:A:221:GLU:CD	1.93	0.70
1:D:263:TRP:C	1:D:263:TRP:CD1	2.65	0.70
1:A:237:PRO:HG2	1:A:240:GLU:HB2	1.75	0.69
1:D:139:SER:O	1:D:143:ASN:HB2	1.93	0.68
1:A:170:SER:OG	2:A:1:NAP:H6N	1.97	0.64
1:C:170:SER:OG	2:C:1:NAP:H6N	1.97	0.64
1:B:271:PRO:O	1:B:275:ILE:HG13	1.99	0.63
1:A:283:SER:H	1:A:284:TYR:HA	1.62	0.63
1:C:92:THR:OG1	1:C:94:GLU:HG3	1.98	0.63
1:B:261:SER:HB3	1:B:264:THR:OG1	1.98	0.63
1:D:274:LYS:O	1:D:278:PHE:CD2	2.52	0.61
1:C:240:GLU:HB2	4:C:324:HOH:O	2.00	0.61
1:A:248:GLY:HA3	1:A:256:VAL:HG21	1.82	0.60
1:C:94:GLU:HB3	4:C:313:HOH:O	2.02	0.60
1:A:133:ILE:HD13	1:B:149:VAL:HG22	1.83	0.59
1:A:273:ARG:O	1:A:277:GLU:HG3	2.02	0.59
1:C:119:ASN:OD1	2:C:1:NAP:H4D	2.03	0.59
1:C:140:MET:HB3	1:D:140:MET:SD	2.42	0.59
1:A:193:PHE:HB2	1:B:185:ALA:HB2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:LEU:HD11	1:C:227:VAL:HG12	1.83	0.59
1:D:170:SER:OG	2:D:1:NAP:H6N	2.03	0.58
1:B:170:SER:HB3	2:B:1:NAP:H5N	1.84	0.58
1:C:223:ALA:O	1:C:227:VAL:HG22	2.03	0.58
1:A:130:HIS:O	1:A:131:ASP:HB2	2.04	0.57
1:B:132:ASP:O	1:B:136:VAL:HG23	2.05	0.56
1:D:39:VAL:HG12	1:D:42:ALA:HB2	1.88	0.56
1:B:273:ARG:O	1:B:277:GLU:HG3	2.05	0.56
1:D:41:GLY:O	1:D:47:GLY:HA3	2.07	0.55
1:C:27:PHE:CG	1:C:247:LYS:HG2	2.41	0.55
1:A:77:HIS:O	1:A:81:LEU:HG	2.06	0.55
1:A:48:ARG:HH22	1:A:73:LYS:HZ2	1.55	0.55
1:B:221:GLU:O	1:B:225:LYS:HG3	2.06	0.55
1:B:171:LEU:HD12	3:B:293:33T:C7	2.37	0.55
1:D:85:SER:O	1:D:86:ALA:HB2	2.06	0.55
1:A:131:ASP:OD1	1:B:152:VAL:HG13	2.07	0.54
1:B:46:ILE:O	1:B:50:MET:HG3	2.06	0.54
1:A:263:TRP:CE3	1:D:263:TRP:HH2	2.25	0.54
1:D:177:TYR:CD1	1:D:178:PRO:HD2	2.43	0.54
1:A:261:SER:O	1:A:265:THR:HG23	2.08	0.53
1:C:140:MET:HE2	1:D:140:MET:HG3	1.90	0.52
1:C:175:VAL:HG11	1:D:276:LEU:CD1	2.39	0.52
1:B:127:ASN:O	1:B:179:MET:HA	2.10	0.52
1:D:144:PHE:O	1:D:147:TYR:HB2	2.10	0.52
1:C:233:MET:O	1:C:234:GLN:CB	2.57	0.52
1:D:119:ASN:OD1	2:D:1:NAP:H4D	2.10	0.52
1:B:93:MET:HG2	2:B:1:NAP:H2A	1.92	0.52
1:D:89:ILE:HD13	1:D:105:GLN:HG3	1.91	0.52
1:D:36:LYS:N	1:D:36:LYS:HD3	2.25	0.52
1:A:62:VAL:HG23	1:A:110:MET:SD	2.49	0.52
1:D:48:ARG:HG3	1:D:74:VAL:HG21	1.92	0.51
1:C:230:ILE:O	1:C:231:VAL:O	2.28	0.51
1:A:56:LYS:HA	1:A:81:LEU:O	2.11	0.51
1:C:157:MET:O	1:C:160:GLN:HB2	2.11	0.51
1:D:180:VAL:O	1:D:180:VAL:HG23	2.09	0.51
1:D:32:LEU:O	1:D:59:ALA:HB2	2.11	0.51
1:B:23:LEU:HD13	1:B:252:ARG:HD3	1.92	0.51
3:A:293:33T:H10	1:B:280[A]:TYR:HE2	1.76	0.50
1:C:43:SER:HB3	1:C:65:ALA:HB3	1.92	0.50
1:D:116:LEU:HD11	1:D:118:LEU:HD21	1.92	0.50
1:C:38:ILE:HG13	1:C:113:LEU:CD1	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:LEU:HD23	1:A:280:TYR:N	2.27	0.50
1:B:62:VAL:N	1:B:110:MET:HE3	2.26	0.50
1:A:216:GLY:HA3	1:A:259:ASP:OD2	2.12	0.50
2:B:1:NAP:H4N	3:B:293:33T:O2	2.12	0.49
1:B:60:HIS:O	1:B:110:MET:HE1	2.11	0.49
1:D:170:SER:HB3	2:D:1:NAP:C5N	2.38	0.49
1:B:62:VAL:HG23	1:B:110:MET:HE3	1.94	0.49
1:C:38:ILE:HG13	1:C:113:LEU:HD11	1.94	0.49
1:D:217:LEU:HD11	1:D:224:MET:CE	2.42	0.49
1:C:236:ALA:HB2	1:C:260:SER:HB3	1.94	0.49
1:D:135:HIS:CD2	4:D:308:HOH:O	2.65	0.49
1:B:52:TYR:CE1	1:B:77:HIS:HB3	2.47	0.49
1:B:97:THR:O	1:B:101:GLN:HG3	2.13	0.49
1:B:109:LEU:N	1:B:109:LEU:HD23	2.28	0.48
1:A:262:LEU:HD12	1:A:262:LEU:O	2.13	0.48
1:A:171:LEU:O	1:A:175:VAL:HG22	2.13	0.48
1:A:276:LEU:HD13	1:B:267:LEU:HD13	1.96	0.48
1:C:248:GLY:HA3	1:C:256:VAL:HG21	1.95	0.48
1:A:269:ARG:NH2	1:A:274:LYS:HE3	2.29	0.48
1:A:186:SER:O	1:A:189:ALA:HB3	2.14	0.48
1:D:122:THR:OG1	1:D:138:LYS:HE3	2.14	0.48
1:D:79:LEU:HD21	1:D:86:ALA:HB3	1.95	0.48
1:D:71:LEU:O	1:D:75:VAL:HG23	2.14	0.48
1:A:36:LYS:HB3	1:A:110:MET:HE3	1.95	0.48
1:D:156:PRO:HB2	4:D:318:HOH:O	2.13	0.48
1:B:124:THR:HG22	1:B:125:SER:N	2.29	0.48
1:B:75:VAL:HG21	1:B:88:TYR:HB3	1.94	0.48
1:A:32:LEU:HD23	1:A:54:LEU:CD2	2.44	0.48
1:D:243:LEU:HG	1:D:247:LYS:HE3	1.96	0.48
1:B:275:ILE:HG12	1:D:266:LEU:HD23	1.95	0.47
1:C:269:ARG:CZ	1:C:274:LYS:NZ	2.77	0.47
1:C:53:HIS:O	1:C:57:MET:HG3	2.15	0.47
1:D:278:PHE:CD2	1:D:278:PHE:N	2.83	0.47
1:C:217:LEU:O	1:C:218:ILE:HD13	2.14	0.47
1:A:55:ALA:HB1	1:A:78:CYS:O	2.14	0.47
1:C:280:TYR:CB	3:D:293:33T:N3	2.78	0.47
1:C:222:THR:HG21	2:C:1:NAP:O2A	2.14	0.47
1:B:68:LYS:HG2	1:B:69:GLU:N	2.29	0.47
1:D:263:TRP:CD1	1:D:264:THR:N	2.83	0.46
1:C:232:HIS:O	1:C:233:MET:HB2	2.15	0.46
1:B:139:SER:O	1:B:143:ASN:HB2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:LEU:HD12	3:B:293:33T:C8	2.46	0.46
1:C:32:LEU:HA	1:C:35:LYS:HG3	1.96	0.46
1:D:145:LEU:HA	1:D:145:LEU:HD12	1.77	0.46
1:B:144:PHE:O	1:B:147:TYR:HB2	2.16	0.46
1:B:77:HIS:O	1:B:81:LEU:HG	2.15	0.46
1:A:169:SER:HB2	1:A:212:LEU:HD11	1.98	0.46
1:B:175:VAL:CG2	1:B:177:TYR:CE2	2.99	0.46
1:A:175:VAL:HG12	1:B:273:ARG:HG3	1.98	0.46
1:D:155:LEU:HG	1:D:159:LYS:HE3	1.98	0.46
1:C:91:GLY:HA3	1:C:98:PHE:CZ	2.50	0.46
1:C:148:VAL:HG12	1:D:133:ILE:CD1	2.46	0.45
1:A:240:GLU:HB3	1:A:258:TYR:OH	2.16	0.45
1:D:217:LEU:HD23	1:D:233:MET:HB2	1.97	0.45
1:C:37:VAL:O	1:C:61:VAL:HA	2.16	0.45
1:A:49:GLU:HG3	1:A:238:LYS:HG3	1.98	0.45
1:A:40:THR:HA	1:A:64:THR:HG22	1.98	0.45
1:A:248:GLY:HA3	1:A:256:VAL:CG2	2.46	0.45
1:C:136:VAL:HG22	1:C:182:ALA:HB2	1.99	0.45
1:B:248:GLY:HA3	1:B:256:VAL:HG21	1.97	0.45
1:B:23:LEU:O	1:B:25:GLU:N	2.49	0.45
1:A:48:ARG:HD3	1:A:74:VAL:HG22	1.99	0.45
1:D:155:LEU:HB3	1:D:156:PRO:HD3	1.99	0.45
1:C:233:MET:O	1:C:234:GLN:HB2	2.17	0.45
1:B:242:ALA:O	1:B:246:ILE:HG13	2.16	0.45
1:D:135:HIS:HD2	4:D:308:HOH:O	2.00	0.45
1:A:276:LEU:HA	1:A:276:LEU:HD12	1.81	0.45
1:C:261:SER:O	1:C:265:THR:HG23	2.18	0.44
1:A:114:ASP:O	1:A:163:GLY:HA3	2.18	0.44
1:D:171:LEU:HG	1:D:216:GLY:HA2	1.98	0.44
1:D:65:ALA:O	1:D:90:ALA:HA	2.17	0.44
1:D:91:GLY:HA3	1:D:98:PHE:CZ	2.52	0.44
1:B:220:THR:HG21	2:B:1:NAP:O2N	2.18	0.44
1:A:170:SER:HB3	2:A:1:NAP:H5N	1.98	0.44
1:A:144:PHE:O	1:A:147:TYR:HB2	2.18	0.44
1:C:145:LEU:HD23	1:D:140:MET:SD	2.58	0.44
1:D:64:THR:HB	1:D:102:PHE:CE1	2.53	0.44
1:A:263:TRP:CZ3	1:D:263:TRP:HH2	2.35	0.43
1:D:236:ALA:HB1	1:D:258:TYR:CE1	2.53	0.43
1:A:68:LYS:O	1:A:72:GLN:HG3	2.18	0.43
1:A:278:PHE:C	1:A:278:PHE:CD2	2.91	0.43
1:A:180:VAL:HG23	1:A:184:SER:OG	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:LEU:HD22	1:B:54:LEU:CD2	2.48	0.43
1:A:139:SER:O	1:A:143:ASN:HB2	2.17	0.43
1:A:194:PHE:HA	1:A:197:ILE:HG12	2.00	0.43
1:B:32:LEU:HD22	1:B:54:LEU:HD23	2.01	0.43
1:B:32:LEU:HD11	1:B:246:ILE:HG22	1.99	0.43
1:B:155:LEU:HG	1:B:159:LYS:HE3	1.99	0.43
1:D:136:VAL:HA	1:D:182:ALA:HB1	2.01	0.43
1:B:42:ALA:HB3	1:B:63:VAL:HB	2.01	0.43
1:D:105:GLN:O	1:D:109:LEU:HD13	2.18	0.43
1:D:62:VAL:HG23	1:D:110:MET:SD	2.59	0.43
1:B:66:ARG:HB2	2:B:1:NAP:O2X	2.18	0.43
1:C:269:ARG:NH1	1:C:274:LYS:HZ3	2.16	0.43
1:C:278:PHE:CD2	1:C:278:PHE:C	2.91	0.43
1:A:43:SER:C	1:A:44:LYS:HG3	2.39	0.43
1:D:114:ASP:OD1	1:D:161:SER:HB2	2.19	0.43
1:D:28:ARG:HA	1:D:29:PRO:HD3	1.87	0.43
1:A:48:ARG:NH2	1:A:73:LYS:HE3	2.34	0.42
1:A:175:VAL:HG23	1:A:177:TYR:CE1	2.54	0.42
1:B:239:GLU:H	1:B:239:GLU:CD	2.22	0.42
1:C:133:ILE:HG23	1:C:134:HIS:N	2.34	0.42
1:A:41:GLY:CA	2:A:1:NAP:H4B	2.49	0.42
1:B:54:LEU:HG	1:B:246:ILE:HD13	2.01	0.42
1:C:175:VAL:HG11	1:D:276:LEU:HD12	2.00	0.42
1:D:88:TYR:O	1:D:89:ILE:HG12	2.19	0.42
1:B:50:MET:HG2	1:B:242:ALA:HB1	2.00	0.42
1:A:130:HIS:O	1:A:131:ASP:CB	2.66	0.42
1:A:272:SER:HB3	1:B:267:LEU:HB3	2.02	0.42
1:C:88:TYR:CD1	1:C:88:TYR:C	2.93	0.42
1:D:278:PHE:HD2	1:D:278:PHE:N	2.18	0.42
1:C:171:LEU:HD12	3:C:293:33T:C7	2.50	0.42
1:B:27:PHE:CD2	1:B:247:LYS:HD3	2.55	0.42
1:C:232:HIS:O	1:C:233:MET:CB	2.68	0.42
1:B:60:HIS:ND1	1:B:85:SER:HB3	2.35	0.42
1:D:62:VAL:HG11	1:D:106:ALA:CB	2.50	0.41
1:A:231:VAL:O	1:A:232:HIS:CB	2.68	0.41
1:A:155:LEU:HG	1:A:159:LYS:HE3	2.02	0.41
1:C:70:THR:O	1:C:74:VAL:HG23	2.20	0.41
1:D:93:MET:HG2	2:D:1:NAP:H2A	2.02	0.41
1:B:120:HIS:CE1	1:B:147:TYR:CE1	3.09	0.41
1:B:213:CYS:SG	1:B:245:ILE:HG23	2.60	0.41
1:D:247:LYS:O	1:D:251:LEU:HG	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:62:VAL:HG11	1:D:106:ALA:HB1	2.03	0.41
1:A:200:GLU:O	1:A:203:VAL:HG22	2.21	0.41
1:B:134:HIS:NE2	1:B:138:LYS:NZ	2.68	0.41
1:C:170:SER:OG	2:C:1:NAP:C6N	2.66	0.41
1:D:269:ARG:NH1	1:D:274:LYS:HE2	2.36	0.41
1:D:263:TRP:C	1:D:263:TRP:HD1	2.23	0.41
1:D:177:TYR:CD2	3:D:293:33T:CL1	3.10	0.41
1:C:224:MET:CE	1:C:235:ALA:HB3	2.50	0.41
1:A:262:LEU:HD12	1:A:266:LEU:HD13	2.03	0.41
1:A:144:PHE:CD2	1:B:140:MET:HE3	2.56	0.41
1:B:172:ALA:HB1	1:B:184:SER:OG	2.20	0.41
1:B:227:VAL:CG1	1:B:227:VAL:O	2.70	0.40
1:C:155:LEU:N	1:C:156:PRO:CD	2.84	0.40
1:D:37:VAL:HG22	1:D:115:MET:HB3	2.04	0.40
1:B:275:ILE:CG1	1:D:266:LEU:HD23	2.50	0.40
1:A:61:VAL:HG12	1:A:63:VAL:HG13	2.03	0.40
1:D:118:LEU:HD22	1:D:150:LEU:HD13	2.03	0.40
1:D:248:GLY:HA3	1:D:256:VAL:HG21	2.02	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	258/286 (90%)	240 (93%)	15 (6%)	3 (1%)	16	11
1	B	260/286 (91%)	242 (93%)	15 (6%)	3 (1%)	16	11
1	C	258/286 (90%)	236 (92%)	19 (7%)	3 (1%)	16	11
1	D	254/286 (89%)	222 (87%)	29 (11%)	3 (1%)	16	11
All	All	1030/1144 (90%)	940 (91%)	78 (8%)	12 (1%)	16	11

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	24	ASN
1	C	231	VAL
1	C	233	MET
1	C	234	GLN
1	D	86	ALA
1	A	232	HIS
1	B	65	ALA
1	B	281	SER
1	A	45	GLY
1	D	69	GLU
1	A	228	SER
1	D	230	ILE

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	206/243 (85%)	197 (96%)	9 (4%)	35	39
1	B	213/243 (88%)	198 (93%)	15 (7%)	19	18
1	C	211/243 (87%)	206 (98%)	5 (2%)	57	67
1	D	206/243 (85%)	193 (94%)	13 (6%)	22	22
All	All	836/972 (86%)	794 (95%)	42 (5%)	31	33

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ARG
1	A	48	ARG
1	A	170	SER
1	A	205	ARG
1	A	221	GLU
1	A	240	GLU
1	A	266	LEU
1	A	276	LEU
1	A	278	PHE
1	B	32	LEU

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Mol	Chain	Res	Type
1	B	61	VAL
1	B	68	LYS
1	B	80	GLU
1	B	85	SER
1	B	131	ASP
1	B	138	LYS
1	B	170	SER
1	B	230	ILE
1	B	261	SER
1	B	265	THR
1	B	269	ARG
1	B	278	PHE
1	B	280[A]	TYR
1	B	280[B]	TYR
1	C	24	ASN
1	C	44	LYS
1	C	88	TYR
1	C	145	LEU
1	C	170	SER
1	D	36	LYS
1	D	70	THR
1	D	100	GLU
1	D	123	ASN
1	D	124	THR
1	D	141	GLU
1	D	170	SER
1	D	233	MET
1	D	263	TRP
1	D	266	LEU
1	D	269	ARG
1	D	276	LEU
1	D	278	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

8 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	NAP	A	1	-	42,52,52	1.54	3 (7%)	54,80,80	1.91	4 (7%)
3	33T	A	293	-	32,33,33	1.58	2 (6%)	47,51,51	1.08	3 (6%)
2	NAP	B	1	-	42,52,52	1.53	3 (7%)	54,80,80	1.85	2 (3%)
3	33T	B	293	-	32,33,33	1.66	2 (6%)	47,51,51	1.01	4 (8%)
2	NAP	C	1	-	42,52,52	1.59	3 (7%)	54,80,80	1.89	2 (3%)
3	33T	C	293	-	32,33,33	1.67	2 (6%)	47,51,51	1.24	5 (10%)
2	NAP	D	1	-	42,52,52	1.56	3 (7%)	54,80,80	1.89	4 (7%)
3	33T	D	293	-	32,33,33	1.56	2 (6%)	47,51,51	1.38	3 (6%)

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	NAP	A	1	-	-	0/27/67/67	0/5/5/5
3	33T	A	293	-	-	0/26/39/39	0/3/3/3
2	NAP	B	1	-	-	0/27/67/67	0/5/5/5
3	33T	B	293	-	-	0/26/39/39	0/3/3/3
2	NAP	C	1	-	-	0/27/67/67	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	33T	C	293	-	-	0/26/39/39	0/3/3/3
2	NAP	D	1	-	-	0/27/67/67	0/5/5/5
3	33T	D	293	-	-	0/26/39/39	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	NAP	C2A-N1A	2.11	1.37	1.33
2	C	1	NAP	C2A-N1A	2.11	1.37	1.33
2	B	1	NAP	C2A-N1A	2.53	1.38	1.33
2	D	1	NAP	C2A-N1A	2.56	1.38	1.33
3	D	293	33T	C12-N3	2.59	1.38	1.33
3	A	293	33T	C12-N3	2.66	1.38	1.33
3	B	293	33T	C12-N3	2.70	1.38	1.33
3	C	293	33T	C12-N3	2.93	1.38	1.33
2	C	1	NAP	C2A-N3A	3.21	1.37	1.32
2	B	1	NAP	C2A-N3A	3.23	1.37	1.32
2	A	1	NAP	C2A-N3A	3.31	1.38	1.32
2	D	1	NAP	C2A-N3A	3.56	1.38	1.32
3	A	293	33T	S1-N2	6.65	1.72	1.63
3	C	293	33T	S1-N2	6.68	1.73	1.63
3	D	293	33T	S1-N2	6.76	1.73	1.63
3	B	293	33T	S1-N2	7.37	1.74	1.63
2	D	1	NAP	O7N-C7N	7.72	1.40	1.24
2	B	1	NAP	O7N-C7N	7.90	1.41	1.24
2	A	1	NAP	O7N-C7N	7.94	1.41	1.24
2	C	1	NAP	O7N-C7N	8.13	1.41	1.24

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	NAP	N3A-C2A-N1A	-11.75	119.90	128.89
2	B	1	NAP	N3A-C2A-N1A	-11.56	120.04	128.89
2	A	1	NAP	N3A-C2A-N1A	-11.54	120.06	128.89
2	C	1	NAP	N3A-C2A-N1A	-11.18	120.33	128.89
3	D	293	33T	C4-C5-N2	-3.28	106.17	109.07
3	C	293	33T	C10-C11-C6	-2.49	118.35	121.36
3	D	293	33T	C10-C11-CL1	-2.28	114.99	118.50
3	A	293	33T	C15-C16-C17	-2.22	120.48	123.35
3	A	293	33T	C11-C6-S1	-2.20	121.86	123.39
3	B	293	33T	C10-C11-C6	-2.11	118.80	121.36
3	C	293	33T	C4-C5-N2	2.03	110.87	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	293	33T	C6-C11-CL1	2.04	123.02	121.54
2	A	1	NAP	C2B-C3B-C4B	2.19	107.04	101.85
3	B	293	33T	C7-C6-C11	2.21	120.60	119.00
3	C	293	33T	C17-C18-C19	2.26	121.54	116.51
2	D	1	NAP	C2N-C3N-C4N	2.34	120.90	118.29
3	C	293	33T	C7-C6-C11	2.54	120.85	119.00
2	A	1	NAP	O4B-C1B-N9A	2.54	113.42	108.10
2	D	1	NAP	O4B-C1B-N9A	2.61	113.57	108.10
3	B	293	33T	C4-C5-N2	2.65	111.42	109.07
2	D	1	NAP	O4D-C1D-N1N	2.72	111.12	108.13
3	A	293	33T	C6-C11-CL1	3.07	123.77	121.54
2	A	1	NAP	O4D-C1D-N1N	3.52	112.00	108.13
2	B	1	NAP	O4D-C1D-N1N	3.59	112.07	108.13
3	C	293	33T	C6-C11-CL1	3.63	124.17	121.54
2	C	1	NAP	O4D-C1D-N1N	4.65	113.25	108.13
3	D	293	33T	C6-C11-CL1	5.56	125.58	121.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	NAP	3	0
3	A	293	33T	1	0
2	B	1	NAP	6	0
3	B	293	33T	3	0
2	C	1	NAP	5	0
3	C	293	33T	1	0
2	D	1	NAP	5	0
3	D	293	33T	2	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 ⓘ

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	260/286 (90%)	-0.06	10 (3%)	44 46	21, 42, 88, 130	2 (0%)
1	B	261/286 (91%)	0.04	14 (5%)	29 31	23, 44, 84, 116	3 (1%)
1	C	260/286 (90%)	0.02	15 (5%)	26 29	20, 39, 85, 127	2 (0%)
1	D	256/286 (89%)	0.15	14 (5%)	29 31	20, 53, 91, 128	6 (2%)
All	All	1037/1144 (90%)	0.04	53 (5%)	32 34	20, 45, 87, 130	13 (1%)

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	262	LEU	5.2
1	C	231	VAL	4.6
1	C	263	TRP	4.3
1	A	263	TRP	4.0
1	C	279	LEU	3.9
1	C	232	HIS	3.6
1	A	229	GLY	3.5
1	A	279	LEU	3.5
1	D	230	ILE	3.5
1	B	229	GLY	3.2
1	B	230	ILE	3.2
1	B	24	ASN	3.1
1	C	24	ASN	3.1
1	A	278	PHE	3.1
1	C	230	ILE	3.1
1	D	280	TYR	3.0
1	B	167	VAL	2.9
1	D	213	CYS	2.9
1	D	231	VAL	2.8
1	B	166	VAL	2.8
1	B	190	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	280[A]	TYR	2.7
1	A	205	ARG	2.7
1	C	283	SER	2.7
1	C	282	THR	2.7
1	A	117	ILE	2.6
1	B	118	LEU	2.6
1	B	168	VAL	2.5
1	D	233	MET	2.5
1	B	282	THR	2.5
1	D	278	PHE	2.4
1	D	188	PHE	2.4
1	C	167	VAL	2.4
1	D	168	VAL	2.3
1	A	203	VAL	2.3
1	A	230	ILE	2.3
1	D	169	SER	2.3
1	A	190	LEU	2.3
1	B	213	CYS	2.2
1	C	203	VAL	2.2
1	C	228	SER	2.2
1	D	263	TRP	2.2
1	B	147	TYR	2.2
1	C	233	MET	2.1
1	D	39	VAL	2.1
1	B	46	ILE	2.1
1	C	229	GLY	2.1
1	A	168	VAL	2.1
1	C	173	GLY	2.1
1	B	169	SER	2.1
1	D	205	ARG	2.0
1	C	278	PHE	2.0
1	D	229	GLY	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 [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	NAP	C	1	48/48	0.98	0.12	-0.14	17,35,57,82	0
2	NAP	A	1	48/48	0.97	0.10	-0.31	18,37,55,58	0
3	33T	D	293	31/31	0.97	0.12	-0.48	33,64,125,128	0
2	NAP	D	1	48/48	0.97	0.10	-0.51	24,47,70,77	0
3	33T	C	293	31/31	0.96	0.12	-0.52	31,63,100,129	0
3	33T	A	293	31/31	0.97	0.10	-0.70	35,55,87,136	0
2	NAP	B	1	48/48	0.98	0.09	-0.73	12,41,73,111	0
3	33T	B	293	31/31	0.98	0.09	-0.75	24,56,105,120	0

6.5 Other polymers [i](#)

There are no such residues in this entry.